Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 03:40 AM UTC

PDB ID	:	5AJ4 / pdb_00005aj4
EMDB ID	:	EMD-2914
Title	:	Structure of the 55S mammalian mitoribosome.
Authors	:	Greber, B.J.; Bieri, P.; Leibundgut, M.; Leitner, A.; Aebersold, R.; Boehringer, D.; Ban, N.
Deposited on	:	2015-02-20
Resolution	:	3.80 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

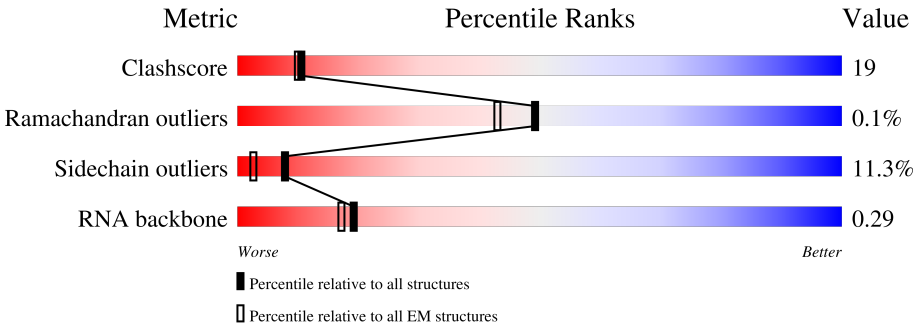
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

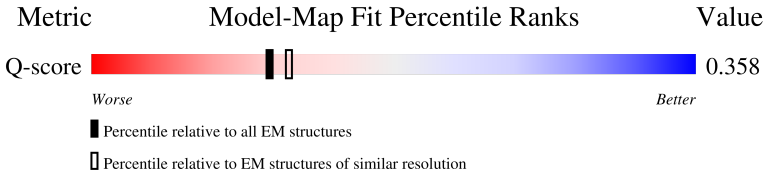
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	10198 (3.30 - 4.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	962	42% 43% 15%
2	AB	220	65% 30% 5%
3	AC	132	5% 53% 39% 8%

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Mol	Chain	Length	Quality of chain
4	AE	328	14% 55% 41%
5	AF	124	6% 64% 28% 6%
6	AG	208	18% 62% 34%
7	AI	311	8% 64% 33%
8	AJ	201	35% 25% 36%
9	AK	136	60% 32% 7%
10	AL	109	63% 29% 7%
11	AN	128	6% 45% 25% 9% 21%
12	AO	239	8% 51% 19% 27%
13	AP	117	10% 62% 35%
14	AQ	109	6% 60% 35% 6%
15	AR	97	65% 28% 7%
16	AU	86	57% 36% 7%
17	AV	69	26% 16% 75% 9%
17	AY	69	35% 23% 57% 20%
18	AX	13	8% 15% 85%
19	Aa	356	16% 47% 33% 18%
20	Ab	190	12% 48% 20% 29%
21	Ac	169	9% 56% 38% 5%
22	Ad	177	5% 69% 27%
23	Ae	336	39% 23% 77%
24	Af	188	30% 21% 47%
25	Ag	397	12% 46% 37% 5% 13%
26	Ah	103	10% 68% 31%
27	Ai	99	6% 68% 28%

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Mol	Chain	Length	Quality of chain
28	Aj	218	36% 59% 36%
29	Ak	275	16% 57% 40%
30	Am	116	20% 66% 30%
31	An	72	62% 28% 8%
32	Ao	530	73% 29% 60% 10%
33	Ap	188	9% 60% 32% 9%
34	As	16	100% 44% 56%
35	Az	17	12% 18% 82%
36	B0	148	43% 28% 6% 23%
37	B1	256	59% 32% 5% 5%
38	B2	252	44% 23% 29%
39	B3	161	43% 24% 6% 27%
40	B4	126	17% 18% 64%
41	B5	188	35% 22% 41%
42	B6	65	60% 34% 28% 12% 26%
43	B7	95	26% 21% 52%
44	B8	188	26% 21% 49%
45	B9	100	18% 18% 62%
46	BA	1570	33% 41% 22%
47	BB	51	29% 55% 12%
48	BD	306	45% 29% 22%
49	BE	348	47% 34% 6% 12%
50	BF	294	44% 34% 6% 15%
51	BI	268	5% 26% 10% 63%
52	BJ	262	10% 37% 25% 36%

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Mol	Chain	Length	Quality of chain
53	BK	192	30% 48% 23% 26%
54	BN	178	49% 42% 8%
55	BO	145	45% 28% 6% 21%
56	BP	296	48% 41% 9%
57	BQ	251	57% 25% 6% 12%
58	BR	169	53% 31% 7% 9%
59	BS	180	37% 38% 21%
60	BT	292	51% 25% 7% 18%
61	BU	149	54% 36% 6%
62	BV	209	41% 30% 26%
63	BW	210	43% 30% 5% 21%
64	BX	150	46% 34% 9% 11%
65	BY	216	16% 56% 31% 7% 6%
66	Ba	423	55% 33% 5% 7%
67	Bb	380	52% 35% 6% 7%
68	Bc	334	51% 33% 12%
69	Bd	206	27% 19% 52%
70	Be	135	52% 35% 10%
71	Bf	142	9% 35% 38% 24%
72	Bg	159	50% 35% 8% 7%
73	Bh	332	52% 33% 13%
74	Bi	312	22% 46% 28% 22%
75	Bj	279	9% 42% 32% 22%
76	Bk	212	6% 42% 20% 36%
77	Bl	166	45% 32% 20%

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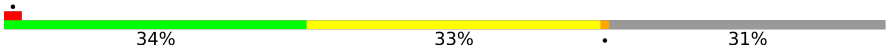
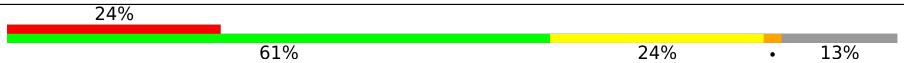
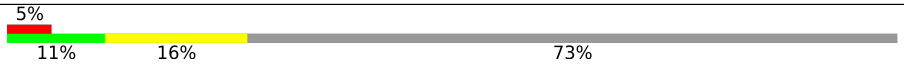
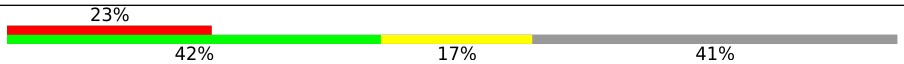
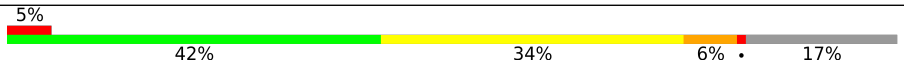
Mol	Chain	Length	Quality of chain
78	Bm	159	
79	Bn	128	
80	Bo	124	
81	Bp	112	
82	Bq	138	
83	Bt	102	
84	Bu	205	
85	Bv	222	
86	Bw	433	
87	Bx	196	
88	Bz	94	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	Y5P	AV	55	-	-	X	-
17	Y5P	AY	55	-	-	X	-
17	Y5P	AY	58	-	-	X	-

2 Entry composition (i)

There are 92 unique types of molecules in this entry. The entry contains 167915 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called MITORIBOSOMAL 12S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	AA	960	20411	9162	3708	6581	960	0	0

- Molecule 2 is a protein called MITORIBOSOMAL PROTEIN US2M, MRPS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	AB	220	1762	1126	326	304	6	0	0

- Molecule 3 is a protein called MITORIBOSOMAL PROTEIN US3M, MRPS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	AC	132	1075	695	195	181	4	0	0

- Molecule 4 is a protein called MITORIBOSOMAL PROTEIN US5M, MRPS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	AE	328	2621	1641	498	471	11	0	0

- Molecule 5 is a protein called MITORIBOSOMAL PROTEIN BS6M, MRPS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	AF	123	990	626	180	178	6	0	0

- Molecule 6 is a protein called MITORIBOSOMAL PROTEIN US7M, MRPS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	AG	208	1721	1097	314	299	11	0	0

- Molecule 7 is a protein called MITORIBOSOMAL PROTEIN US9M, MRPS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AI	311	Total	C	N	O	S	0	0
			2498	1586	450	449	13		

- Molecule 8 is a protein called MITORIBOSOMAL PROTEIN US10M, MRPS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AJ	129	Total	C	N	O	S	0	0
			1067	690	182	192	3		

- Molecule 9 is a protein called MITORIBOSOMAL PROTEIN US11M, MRPS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AK	136	Total	C	N	O	S	0	0
			1001	628	192	178	3		

- Molecule 10 is a protein called MITORIBOSOMAL PROTEIN US12M, MRPS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AL	109	Total	C	N	O	S	0	0
			840	524	172	138	6		

- Molecule 11 is a protein called MITORIBOSOMAL PROTEIN US14M, MRPS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AN	101	Total	C	N	O	S	0	0
			858	534	174	144	6		

- Molecule 12 is a protein called MITORIBOSOMAL PROTEIN US15M, MRPS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AO	175	Total	C	N	O	S	0	0
			1448	919	272	248	9		

- Molecule 13 is a protein called MITORIBOSOMAL PROTEIN BS16M, MRPS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AP	117	Total	C	N	O	S	0	0
			932	588	184	155	5		

- Molecule 14 is a protein called MITORIBOSOMAL PROTEIN US17M, MRPS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AQ	109	Total	C	N	O	S	0	0
			853	555	150	145	3		

- Molecule 15 is a protein called MITORIBOSOMAL PROTEIN BS18M, MRPS18C.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AR	97	Total	C	N	O	S	0	0
			784	507	132	138	7		

- Molecule 16 is a protein called MITORIBOSOMAL PROTEIN BS21M, MRPS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AU	86	Total	C	N	O	S	0	0
			734	453	148	125	8		

- Molecule 17 is a RNA chain called P-SITE AND A-SITE TRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AV	69	Total	C	N	O	P	0	0
			1251	625	146	412	68		
17	AY	69	Total	C	N	O	P	0	0
			1251	625	146	412	68		

- Molecule 18 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AX	13	Total	C	N	O	P	0	0
			231	117	26	76	12		

- Molecule 19 is a protein called MITORIBOSOMAL PROTEIN MS22, MRPS22.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Aa	292	Total	C	N	O	S	0	0
			2296	1476	394	417	9		

- Molecule 20 is a protein called MITORIBOSOMAL PROTEIN MS23, MRPS23.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Ab	135	Total	C	N	O	S	0	0
			1101	709	199	192	1		

- Molecule 21 is a protein called MITORIBOSOMAL PROTEIN MS25, MRPS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Ac	169	Total	C	N	O	S	0	0
			1367	876	236	245	10		

- Molecule 22 is a protein called MITORIBOSOMAL PROTEIN MS26, MRPS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Ad	177	Total	C	N	O	S	0	0
			1467	904	288	273	2		

- Molecule 23 is a protein called MITORIBOSOMAL PROTEIN MS27, MRPS27.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	Ae	336	Total	C	N	O	0	0
			2016	1344	336	336		

- Molecule 24 is a protein called MITORIBOSOMAL PROTEIN MS28, MRPS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Af	99	Total	C	N	O	S	0	0
			778	494	134	146	4		

- Molecule 25 is a protein called MITORIBOSOMAL PROTEIN MS29, MRPS29.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Ag	346	Total	C	N	O	S	0	0
			2774	1786	489	489	10		

- Molecule 26 is a protein called MITORIBOSOMAL PROTEIN MS31, MRPS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Ah	103	Total	C	N	O	S	0	0
			876	569	145	159	3		

- Molecule 27 is a protein called MITORIBOSOMAL PROTEIN MS33, MRPS33.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Ai	99	Total	C	N	O	S	0	0
			824	522	156	143	3		

- Molecule 28 is a protein called MITORIBOSOMAL PROTEIN MS34, MRPS34.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Aj	213	Total	C	N	O	S	0	0
			1777	1123	339	308	7		

- Molecule 29 is a protein called MITORIBOSOMAL PROTEIN MS35, MRPS35.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Ak	275	Total	C	N	O	S	0	0
			2222	1414	380	419	9		

- Molecule 30 is a protein called MITORIBOSOMAL PROTEIN MS37, MRPS37.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Am	116	Total	C	N	O	S	0	0
			930	577	185	160	8		

- Molecule 31 is a protein called MITORIBOSOMAL PROTEIN MS38, MRPS38.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	An	72	Total	C	N	O	S	0	0
			639	407	139	92	1		

- Molecule 32 is a protein called MITORIBOSOMAL PROTEIN MS39, MRPS39.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Ao	476	Total	C	N	O	S	0	0
			3028	2007	500	519	2		

- Molecule 33 is a protein called 28S RIBOSOMAL PROTEIN S18B, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Ap	188	Total	C	N	O	S	0	0
			1551	983	290	270	8		

- Molecule 34 is a protein called UNASSIGNED HELICES.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	As	16	Total	C	N	O	0	0
			96	64	16	16		

- Molecule 35 is a protein called UNASSIGNED HELICES.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	Az	17	Total	C	N	O	0	0
			102	68	17	17		

- Molecule 36 is a protein called MITORIBOSOMAL PROTEIN BL27M, MRPL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	B0	114	Total	C	N	O	S	0	0
			878	564	160	151	3		

- Molecule 37 is a protein called MITORIBOSOMAL PROTEIN BL28M, MRPL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	B1	244	Total	C	N	O	S	0	0
			2036	1315	363	353	5		

- Molecule 38 is a protein called MITORIBOSOMAL PROTEIN UL29M, MRPL47.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	B2	178	Total	C	N	O	S	0	0
			1544	990	289	259	6		

- Molecule 39 is a protein called MITORIBOSOMAL PROTEIN UL30M, MRPL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	B3	118	Total	C	N	O	S	0	0
			968	622	178	165	3		

- Molecule 40 is a protein called MITORIBOSOMAL PROTEIN BL31M, MRPL55.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	B4	45	Total	C	N	O	S	0	0
			381	239	77	62	3		

- Molecule 41 is a protein called MITORIBOSOMAL PROTEIN BL32M, MRPL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	B5	110	Total	C	N	O	S	0	0
			902	553	181	162	6		

- Molecule 42 is a protein called MITORIBOSOMAL PROTEIN BL33M, MRPL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	B6	48	Total	C	N	O	S	0	0
			391	253	70	66	2		

- Molecule 43 is a protein called MITORIBOSOMAL PROTEIN BL34M, MRPL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	B7	46	Total	C	N	O	S	0	0
			387	239	89	58	1		

- Molecule 44 is a protein called MITORIBOSOMAL PROTEIN BL35M, MRPL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	B8	95	Total	C	N	O	S	0	0
			833	539	163	129	2		

- Molecule 45 is a protein called MITORIBOSOMAL PROTEIN BL36M, MRPL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	B9	38	Total	C	N	O	S	0	0
			335	214	70	47	4		

- Molecule 46 is a RNA chain called MITORIBOSOMAL 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BA	1515	Total	C	N	O	P	0	0
			32233	14473	5860	10385	1515		

- Molecule 47 is a RNA chain called MITORIBOSOMAL CP TRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BB	51	Total	C	N	O	P	0	0
			1008	489	162	306	51		

- Molecule 48 is a protein called MITORIBOSOMAL PROTEIN UL2M, MRPL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BD	240	Total	C	N	O	S	0	0
			1860	1160	371	319	10		

- Molecule 49 is a protein called MITORIBOSOMAL PROTEIN UL3M, MRPL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BE	307	Total	C	N	O	S	0	0
			2420	1554	426	430	10		

- Molecule 50 is a protein called MITORIBOSOMAL PROTEIN UL4M, MRPL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BF	250	Total	C	N	O	S	0	0
			2011	1294	367	344	6		

- Molecule 51 is a protein called MITORIBOSOMAL PROTEIN BL9M, MRPL9.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	BI	98	Total	C	N	O	0	0
			805	509	155	141		

- Molecule 52 is a protein called MITORIBOSOMAL PROTEIN UL10M, MRPL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	BJ	168	Total	C	N	O	S	0	0
			1361	879	248	226	8		

- Molecule 53 is a protein called MITORIBOSOMAL PROTEIN UL11M, MRPL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BK	142	Total	C	N	O	S	0	0
			1081	690	197	192	2		

- Molecule 54 is a protein called MITORIBOSOMAL PROTEIN UL13M, MRPL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	BN	177	Total	C	N	O	S	0	0
			1444	926	258	253	7		

- Molecule 55 is a protein called MITORIBOSOMAL PROTEIN UL14M, MRPL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	BO	115	Total	C	N	O	S	0	0
			896	562	176	154	4		

- Molecule 56 is a protein called MITORIBOSOMAL PROTEIN UL15M, MRPL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	BP	288	Total	C	N	O	S	0	0
			2312	1473	430	403	6		

- Molecule 57 is a protein called MITORIBOSOMAL PROTEIN UL16M, MRPL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	BQ	221	Total	C	N	O	S	0	0
			1792	1147	330	305	10		

- Molecule 58 is a protein called MITORIBOSOMAL PROTEIN BL17M, MRPL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	BR	153	Total	C	N	O	S	0	0
			1240	777	236	222	5		

- Molecule 59 is a protein called MITORIBOSOMAL PROTEIN UL18M, MRPL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	BS	143	Total	C	N	O	S	0	0
			1168	733	227	204	4		

- Molecule 60 is a protein called MITORIBOSOMAL PROTEIN BL19M, MRPL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	BT	239	Total	C	N	O	S	0	0
			1950	1249	339	353	9		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BT	54	UNK	PHE	conflict	UNP I3LNJ0
BT	55	UNK	GLN	conflict	UNP I3LNJ0
BT	56	UNK	PRO	conflict	UNP I3LNJ0
BT	57	UNK	PRO	conflict	UNP I3LNJ0
BT	58	UNK	PRO	conflict	UNP I3LNJ0
BT	59	UNK	LYS	conflict	UNP I3LNJ0
BT	60	UNK	PRO	conflict	UNP I3LNJ0
BT	61	UNK	VAL	conflict	UNP I3LNJ0
BT	62	UNK	ILE	conflict	UNP I3LNJ0
BT	63	UNK	VAL	conflict	UNP I3LNJ0
BT	64	UNK	ASP	conflict	UNP I3LNJ0
BT	65	UNK	LYS	conflict	UNP I3LNJ0

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Chain	Residue	Modelled	Actual	Comment	Reference
BT	66	UNK	ARG	conflict	UNP I3LNJ0
BT	67	UNK	ARG	conflict	UNP I3LNJ0
BT	68	UNK	PRO	conflict	UNP I3LNJ0

- Molecule 61 is a protein called MITORIBOSOMAL PROTEIN BL20M, MRPL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	BU	140	Total	C	N	O	S	0	0
			1159	732	239	185	3		

- Molecule 62 is a protein called MITORIBOSOMAL PROTEIN BL21M, MRPL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	BV	155	Total	C	N	O	S	0	0
			1231	789	219	219	4		

- Molecule 63 is a protein called MITORIBOSOMAL PROTEIN UL22M, MRPL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	BW	166	Total	C	N	O	S	0	0
			1374	876	258	234	6		

- Molecule 64 is a protein called MITORIBOSOMAL PROTEIN UL23M, MRPL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	BX	134	Total	C	N	O	S	0	0
			1120	715	217	186	2		

- Molecule 65 is a protein called MITORIBOSOMAL PROTEIN UL24M, MRPL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	BY	204	Total	C	N	O	S	0	0
			1663	1047	305	306	5		

- Molecule 66 is a protein called MITORIBOSOMAL PROTEIN ML37, MRPL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	Ba	393	Total	C	N	O	S	0	0
			3173	2040	556	565	12		

- Molecule 67 is a protein called MITORIBOSOMAL PROTEIN ML38, MRPL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	Bb	354	Total	C	N	O	S	0	0
			2952	1876	542	525	9		

- Molecule 68 is a protein called MITORIBOSOMAL PROTEIN ML39, MRPL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Bc	295	Total	C	N	O	S	0	0
			2408	1541	410	441	16		

- Molecule 69 is a protein called MITORIBOSOMAL PROTEIN ML40, MRPL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Bd	99	Total	C	N	O	S	0	0
			832	528	148	155	1		

- Molecule 70 is a protein called MITORIBOSOMAL PROTEIN ML41, MRPL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Be	121	Total	C	N	O	S	0	0
			968	626	167	172	3		

- Molecule 71 is a protein called MITORIBOSOMAL PROTEIN ML42, MRPL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Bf	108	Total	C	N	O	S	0	0
			852	544	154	150	4		

- Molecule 72 is a protein called MITORIBOSOMAL PROTEIN ML43, MRPL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Bg	148	Total	C	N	O	S	0	0
			1167	727	225	212	3		

- Molecule 73 is a protein called MITORIBOSOMAL PROTEIN ML44, MRPL44.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Bh	289	Total	C	N	O	S	0	0
			2319	1486	399	426	8		

- Molecule 74 is a protein called MITORIBOSOMAL PROTEIN ML45, MRPL45.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Bi	242	Total	C	N	O	S	0	0
			1979	1266	352	351	10		

- Molecule 75 is a protein called MITORIBOSOMAL PROTEIN ML46, MRPL46.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Bj	217	Total	C	N	O	S	0	0
			1775	1137	311	321	6		

- Molecule 76 is a protein called MITORIBOSOMAL PROTEIN ML48, MRPL48.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Bk	136	Total	C	N	O	S	0	0
			1087	692	185	205	5		

- Molecule 77 is a protein called MITORIBOSOMAL PROTEIN ML49, MRPL49.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Bl	133	Total	C	N	O	S	0	0
			1097	709	192	194	2		

- Molecule 78 is a protein called MITORIBOSOMAL PROTEIN ML50, MRPL50.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Bm	109	Total	C	N	O	S	0	0
			893	568	160	162	3		

- Molecule 79 is a protein called MITORIBOSOMAL PROTEIN ML51, MRPL51.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Bn	97	Total	C	N	O	S	0	0
			837	539	166	128	4		

- Molecule 80 is a protein called MITORIBOSOMAL PROTEIN ML52, MRPL52.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Bo	94	Total	C	N	O	S	0	0
			747	466	143	136	2		

- Molecule 81 is a protein called MITORIBOSOMAL PROTEIN ML53, MRPL53.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Bp	97	Total	C	N	O	S	0	0
			742	459	143	134	6		

- Molecule 82 is a protein called MITORIBOSOMAL PROTEIN ML54, MRPL54.

Mol	Chain	Residues	Atoms				AltConf	Trace
82	Bq	37	Total	C	N	O	0	0
			336	214	69	53		

- Molecule 83 is a protein called MITORIBOSOMAL PROTEIN ML63, MRPL57.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	Bt	94	Total	C	N	O	S	0	0
			780	485	168	126	1		

- Molecule 84 is a protein called MITORIBOSOMAL PROTEIN ML62, MRPL58.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	Bu	151	Total	C	N	O	S	0	0
			1208	748	233	222	5		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Bu	164	UNK	ALA	conflict	UNP W5IDC0
Bu	165	UNK	LYS	conflict	UNP W5IDC0
Bu	166	UNK	GLU	conflict	UNP W5IDC0
Bu	167	UNK	PRO	conflict	UNP W5IDC0
Bu	168	UNK	SER	conflict	UNP W5IDC0
Bu	169	UNK	ARG	conflict	UNP W5IDC0
Bu	170	UNK	GLU	conflict	UNP W5IDC0
Bu	171	UNK	ASP	conflict	UNP W5IDC0
Bu	172	UNK	ALA	conflict	UNP W5IDC0
Bu	173	UNK	GLU	conflict	UNP W5IDC0

- Molecule 85 is a protein called MITORIBOSOMAL PROTEIN ML64, MRPL59.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	Bv	131	Total	C	N	O	S	0	0
			1068	662	206	195	5		

- Molecule 86 is a protein called MITORIBOSOMAL PROTEIN ML65, MRPS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	Bw	387	Total 3126	C 2011	N 548	O 555	S 12	0	0

- Molecule 87 is a protein called MITORIBOSOMAL PROTEIN ML66, MRPS18A.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	Bx	162	Total 1325	C 845	N 249	O 224	S 7	0	0

- Molecule 88 is a protein called UNASSIGNED SECONDARY STRUCTURE ELEMENTS.

Mol	Chain	Residues	Atoms				AltConf	Trace
88	Bz	94	Total 564	C 376	N 94	O 94	0	0

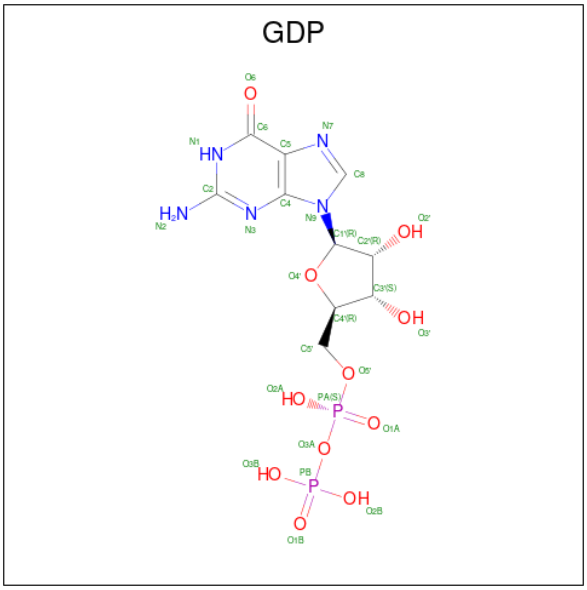
- Molecule 89 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
89	AA	146	Total 146	Mg 146	0
89	Ag	1	Total 1	Mg 1	0
89	B0	1	Total 1	Mg 1	0
89	B2	1	Total 1	Mg 1	0
89	BA	195	Total 195	Mg 195	0
89	BD	2	Total 2	Mg 2	0
89	BE	1	Total 1	Mg 1	0
89	BP	1	Total 1	Mg 1	0
89	BR	2	Total 2	Mg 2	0
89	BX	1	Total 1	Mg 1	0

- Molecule 90 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
90	AR	1	Total Zn 1 1	0
90	Ac	1	Total Zn 1 1	0
90	Ap	1	Total Zn 1 1	0
90	B5	1	Total Zn 1 1	0
90	B9	1	Total Zn 1 1	0
90	Bx	1	Total Zn 1 1	0

- Molecule 91 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms	AltConf
91	Ag	1	Total C N O P 28 10 5 11 2	0

- Molecule 92 is water.

Mol	Chain	Residues	Atoms	AltConf
92	AA	114	Total O 114 114	0
92	Ag	4	Total O 4 4	0
92	B0	3	Total O 3 3	0

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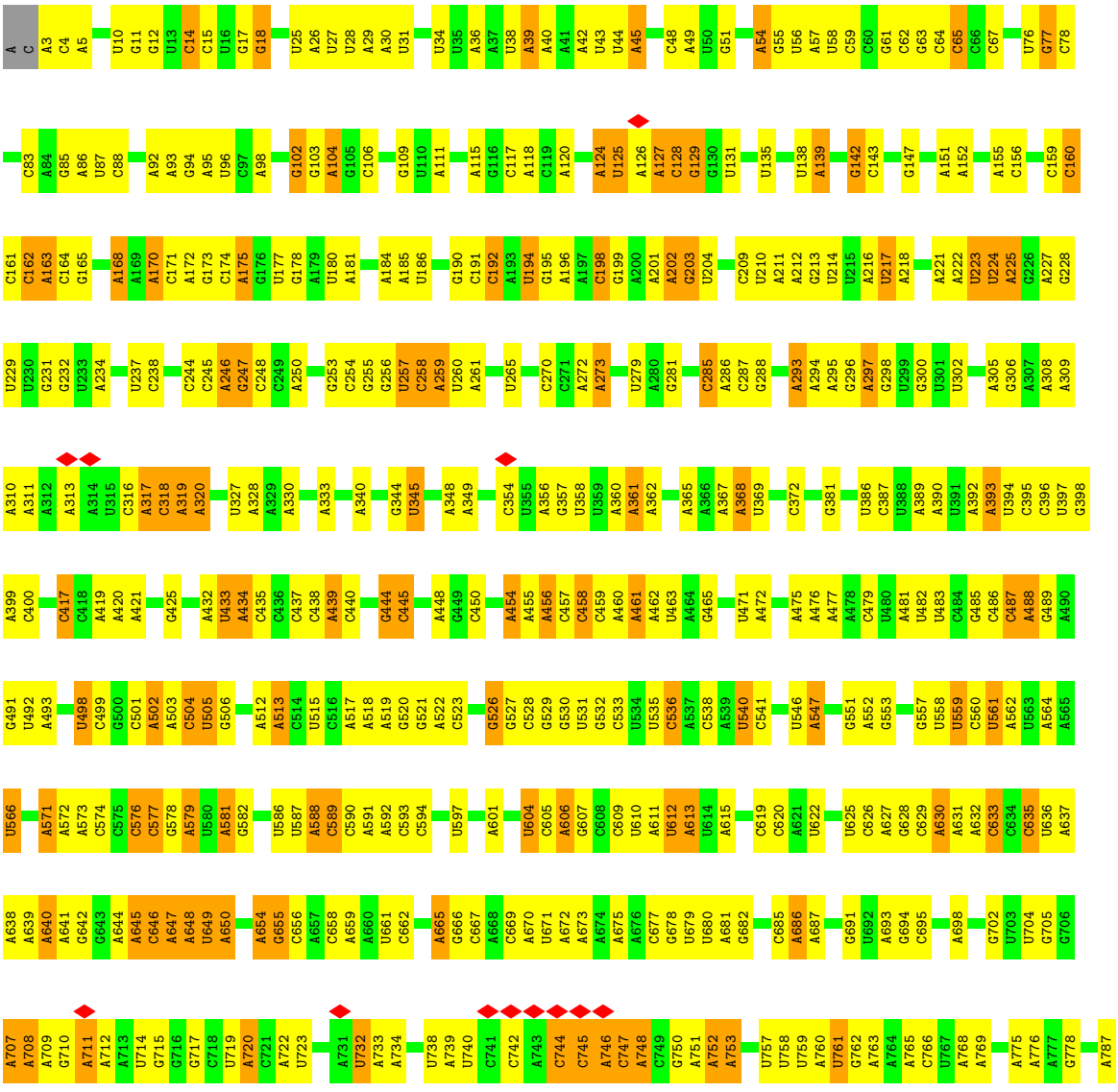
Mol	Chain	Residues	Atoms	AltConf
92	B7	2	Total O 2 2	0
92	B8	1	Total O 1 1	0
92	BA	196	Total O 196 196	0
92	BD	3	Total O 3 3	0
92	BF	4	Total O 4 4	0
92	BI	1	Total O 1 1	0
92	BO	2	Total O 2 2	0
92	BP	3	Total O 3 3	0
92	BR	2	Total O 2 2	0
92	BU	1	Total O 1 1	0
92	BW	4	Total O 4 4	0

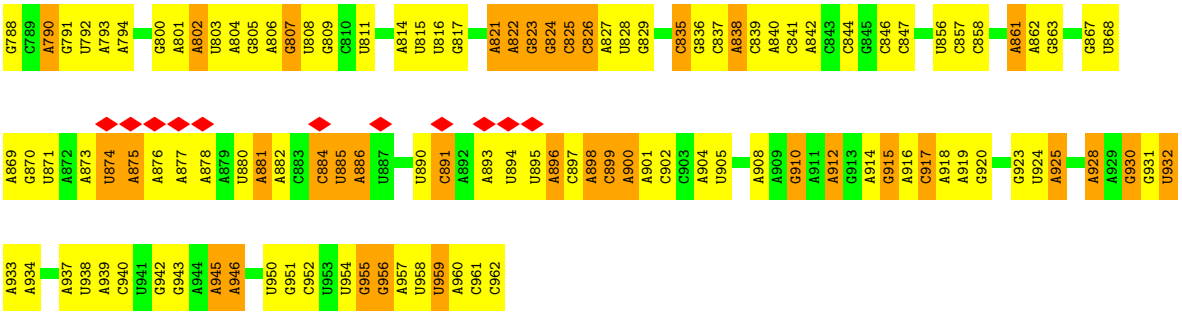
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: MITORIBOSOMAL 12S Ribosomal RNA

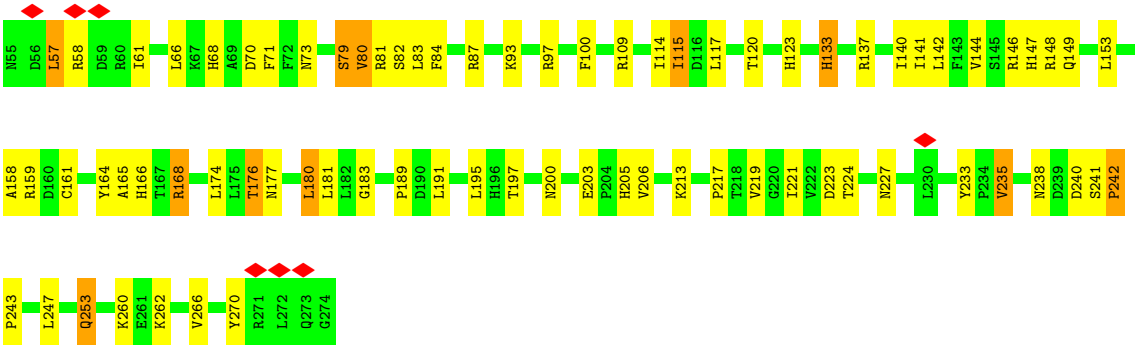
Chain AA:





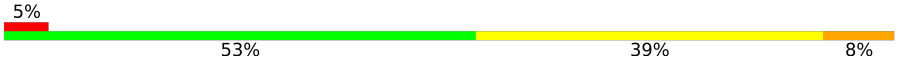
• Molecule 2: MITORIBOSOMAL PROTEIN US2M, MRPS2

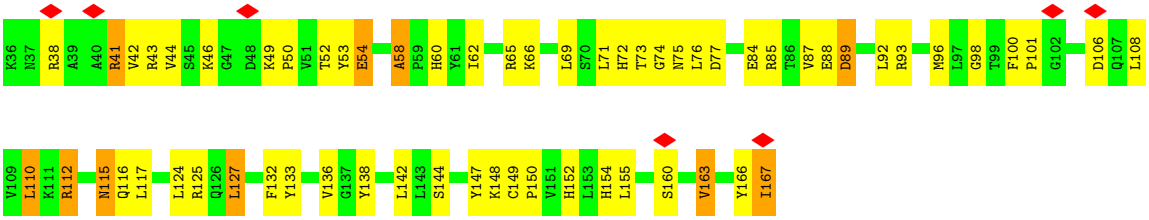
Chain AB:



• Molecule 3: MITORIBOSOMAL PROTEIN US3M, MRPS24

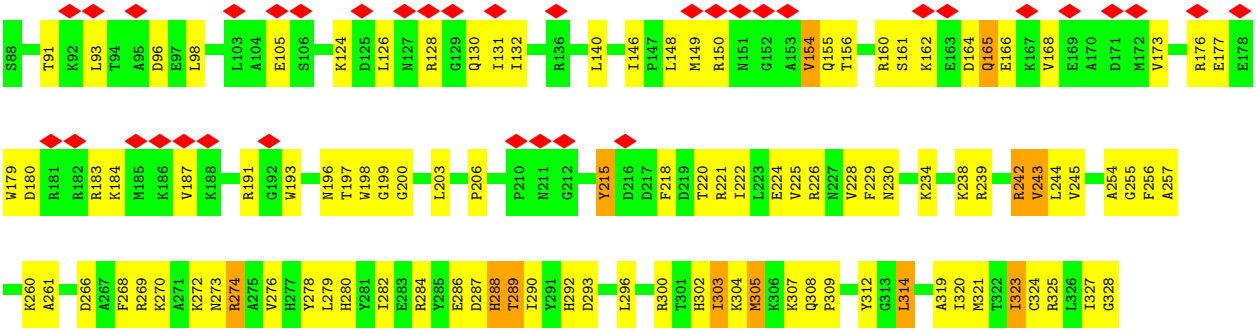
Chain AC:

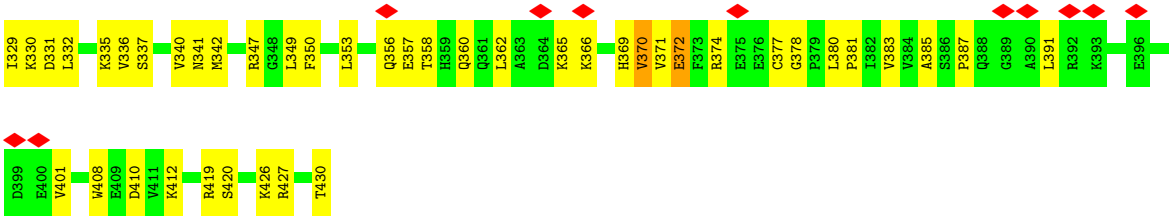




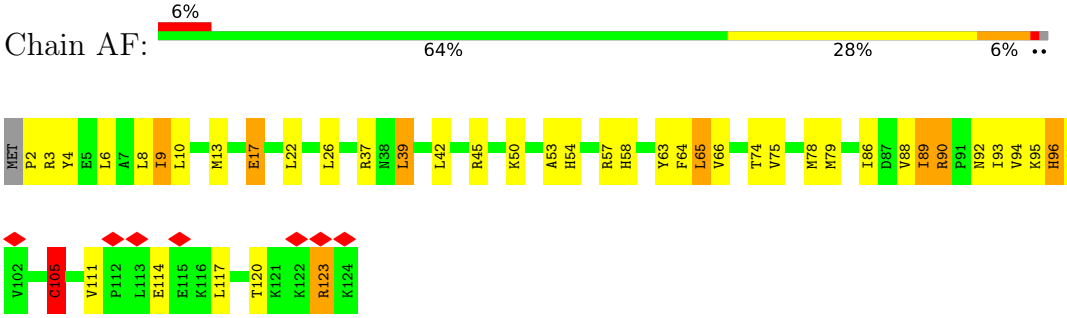
• Molecule 4: MITORIBOSOMAL PROTEIN US5M, MRPS5

Chain AE:

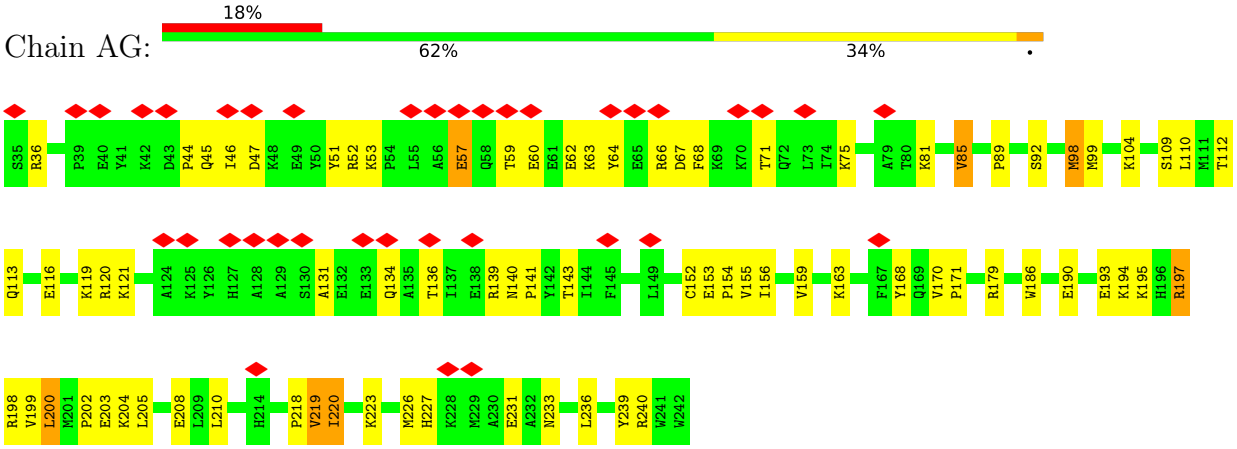




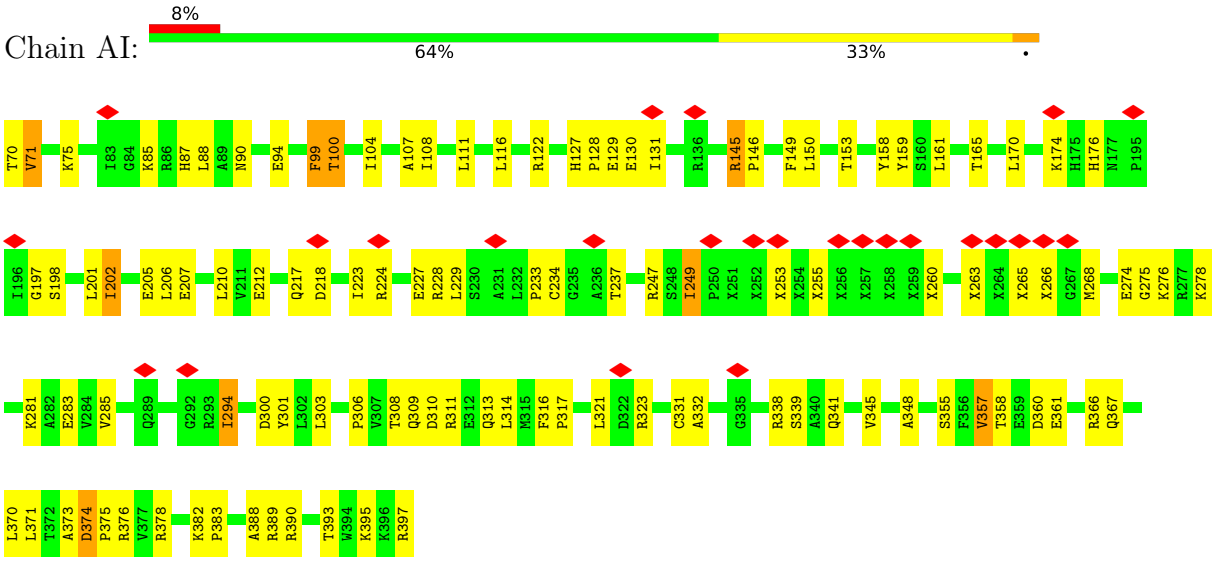
• Molecule 5: MITORIBOSOMAL PROTEIN BS6M, MRPS6



• Molecule 6: MITORIBOSOMAL PROTEIN US7M, MRPS7

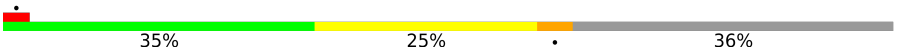


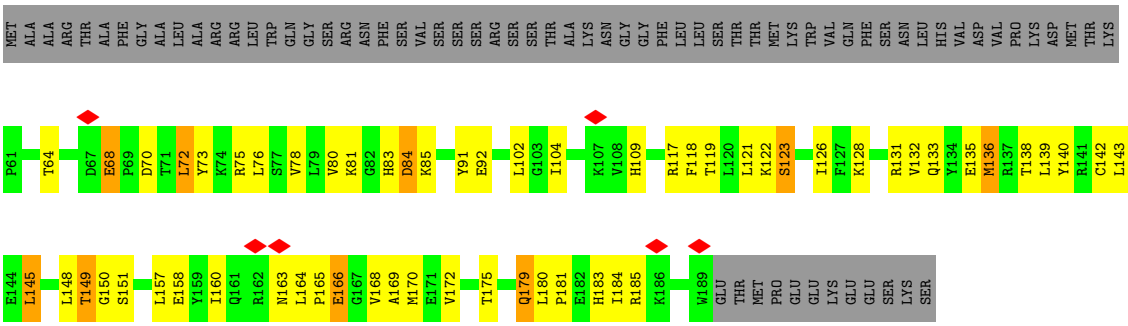
• Molecule 7: MITORIBOSOMAL PROTEIN US9M, MRPS9



• Molecule 8: MITORIBOSOMAL PROTEIN US10M, MRPS10

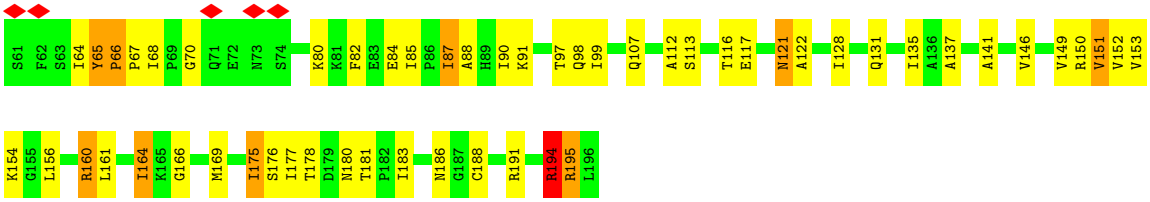
Chain AJ:





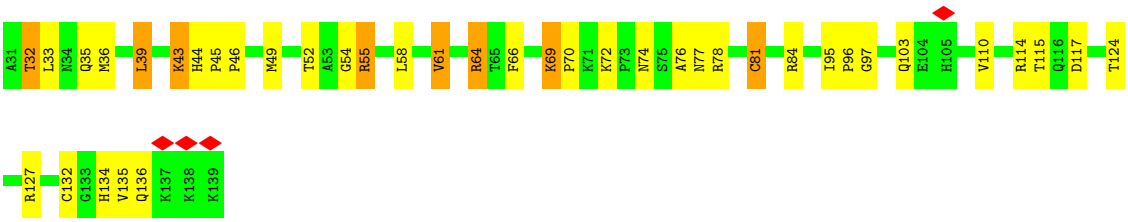
• Molecule 9: MITORIBOSOMAL PROTEIN US11M, MRPS11

Chain AK:



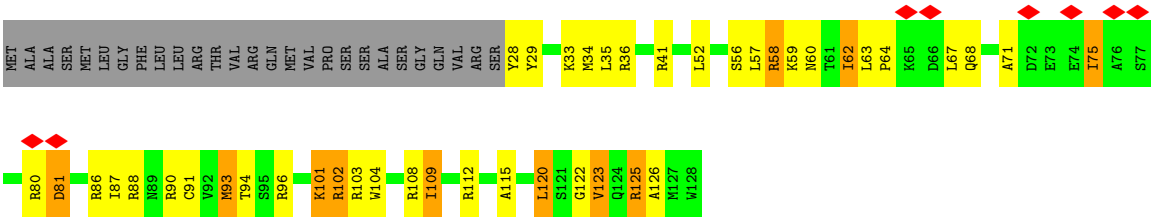
• Molecule 10: MITORIBOSOMAL PROTEIN US12M, MRPS12

Chain AL:



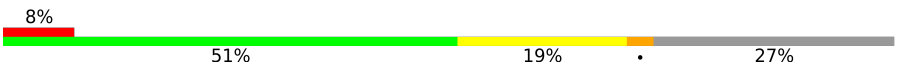
• Molecule 11: MITORIBOSOMAL PROTEIN US14M, MRPS14

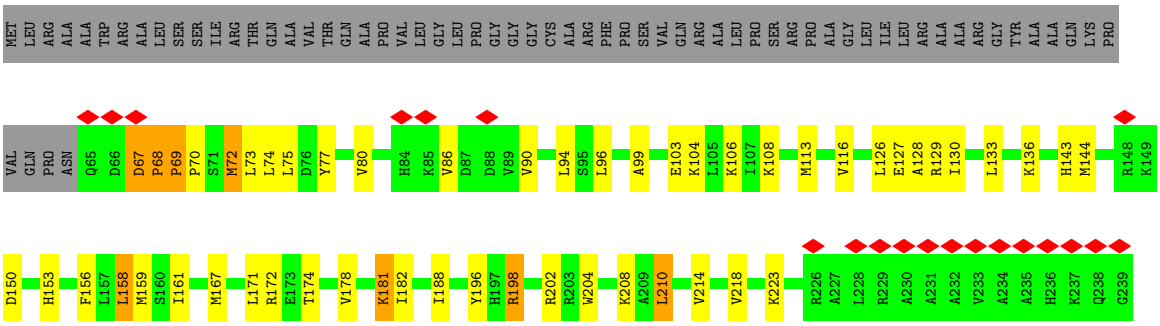
Chain AN:



• Molecule 12: MITORIBOSOMAL PROTEIN US15M, MRPS15

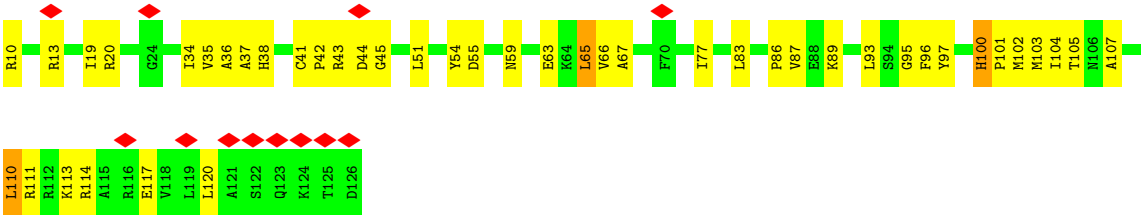
Chain AO:





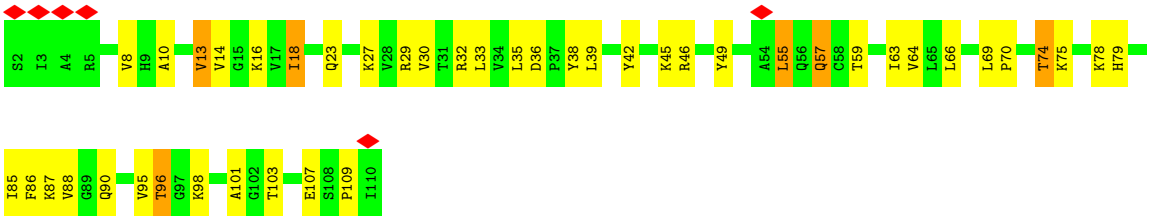
• Molecule 13: MITORIBOSOMAL PROTEIN BS16M, MRPS16

Chain AP:



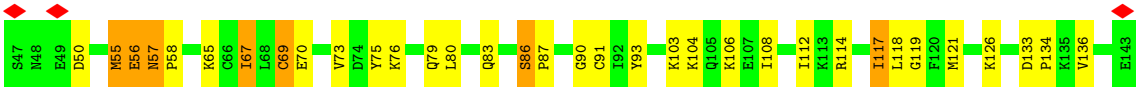
• Molecule 14: MITORIBOSOMAL PROTEIN US17M, MRPS17

Chain AQ:



• Molecule 15: MITORIBOSOMAL PROTEIN BS18M, MRPS18C

Chain AR:

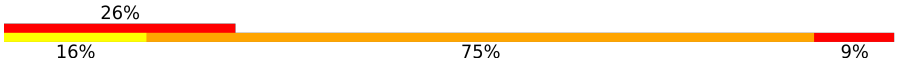


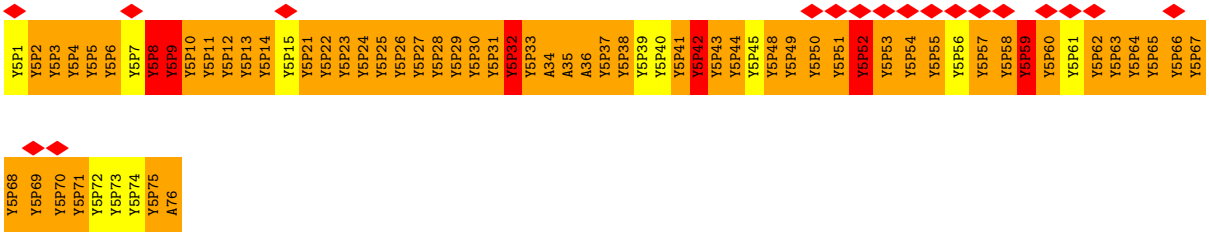
• Molecule 16: MITORIBOSOMAL PROTEIN BS21M, MRPS21

Chain AU:

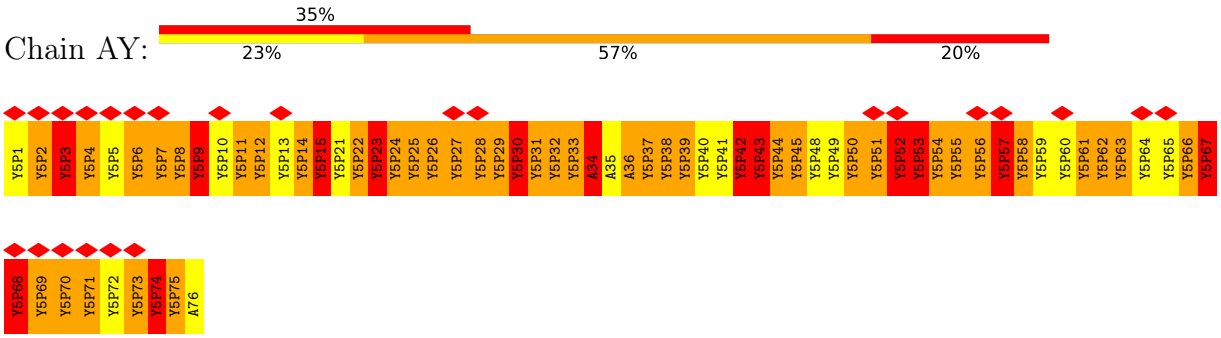
• Molecule 17: P-SITE AND A-SITE TRNA

Chain AV:



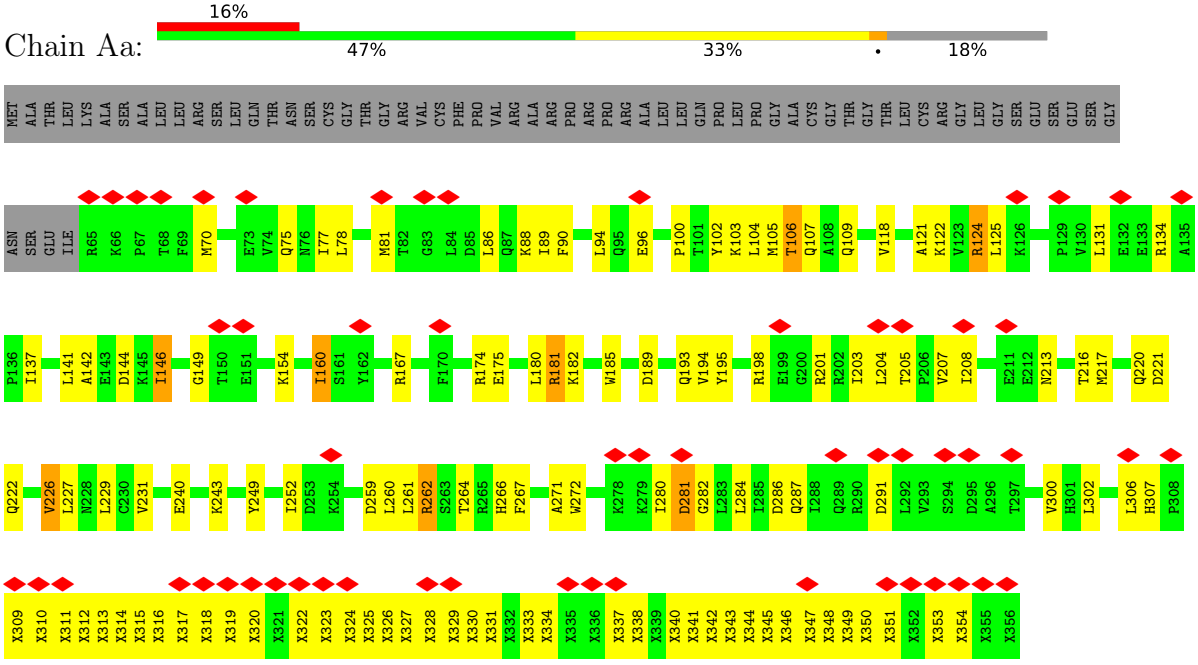


• Molecule 17: P-SITE AND A-SITE TRNA



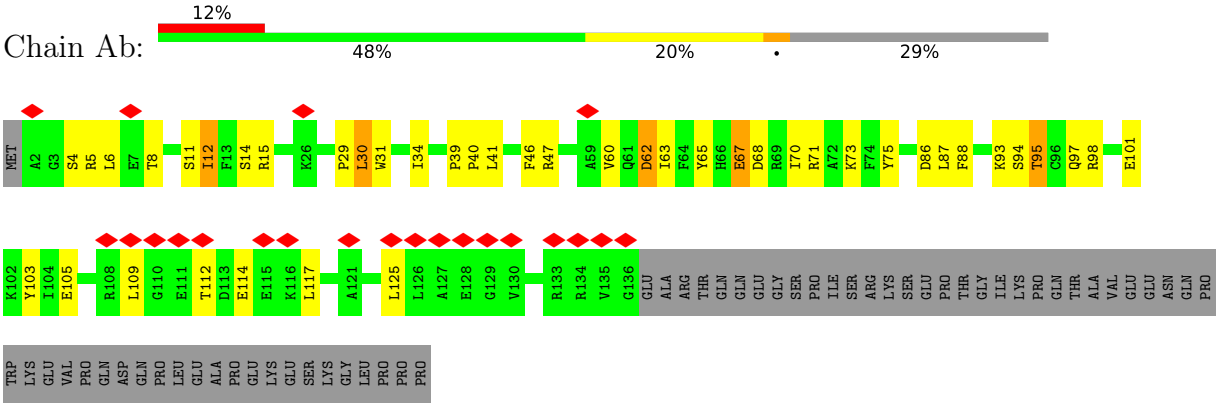
• Molecule 18: MRNA

• Molecule 19: MITORIBOSOMAL PROTEIN MS22, MRPS22



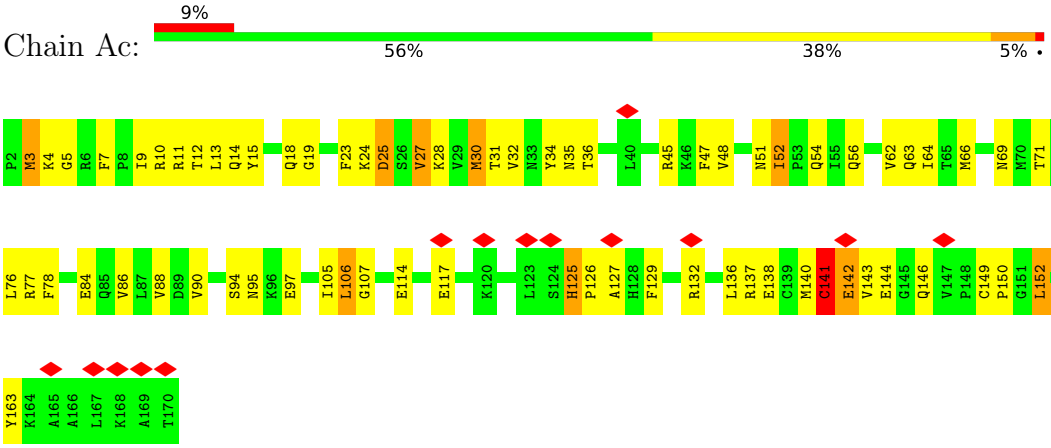
• Molecule 20: MITORIBOSOMAL PROTEIN MS23, MRPS23

Chain Ab:



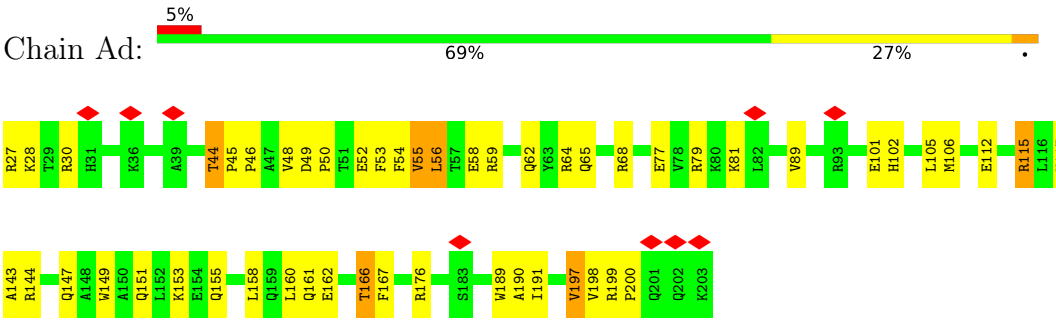
• Molecule 21: MITORIBOSOMAL PROTEIN MS25, MRPS25

Chain Ac:



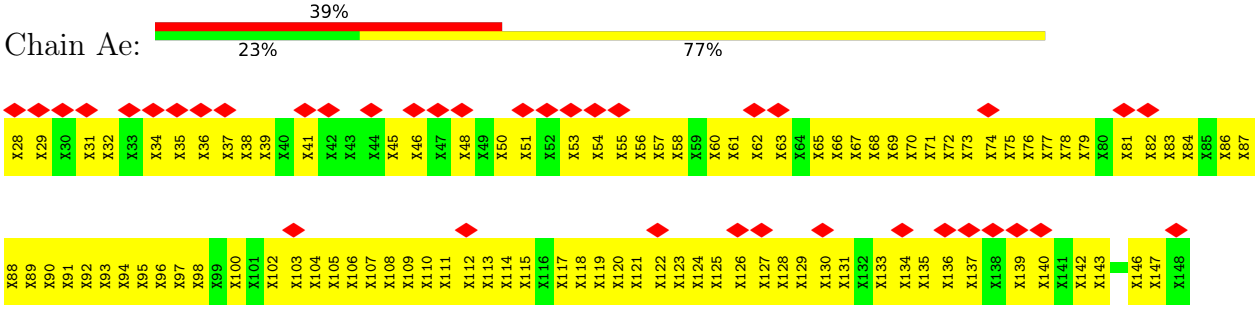
• Molecule 22: MITORIBOSOMAL PROTEIN MS26, MRPS26

Chain Ad:



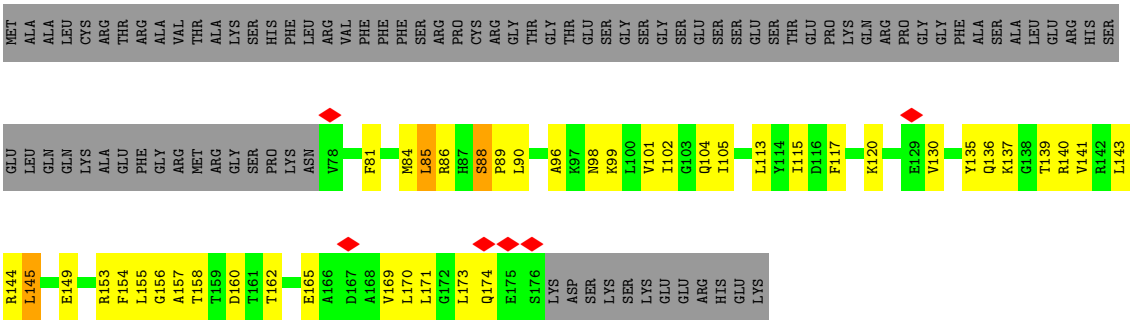
• Molecule 23: MITORIBOSOMAL PROTEIN MS27, MRPS27

Chain Ae:



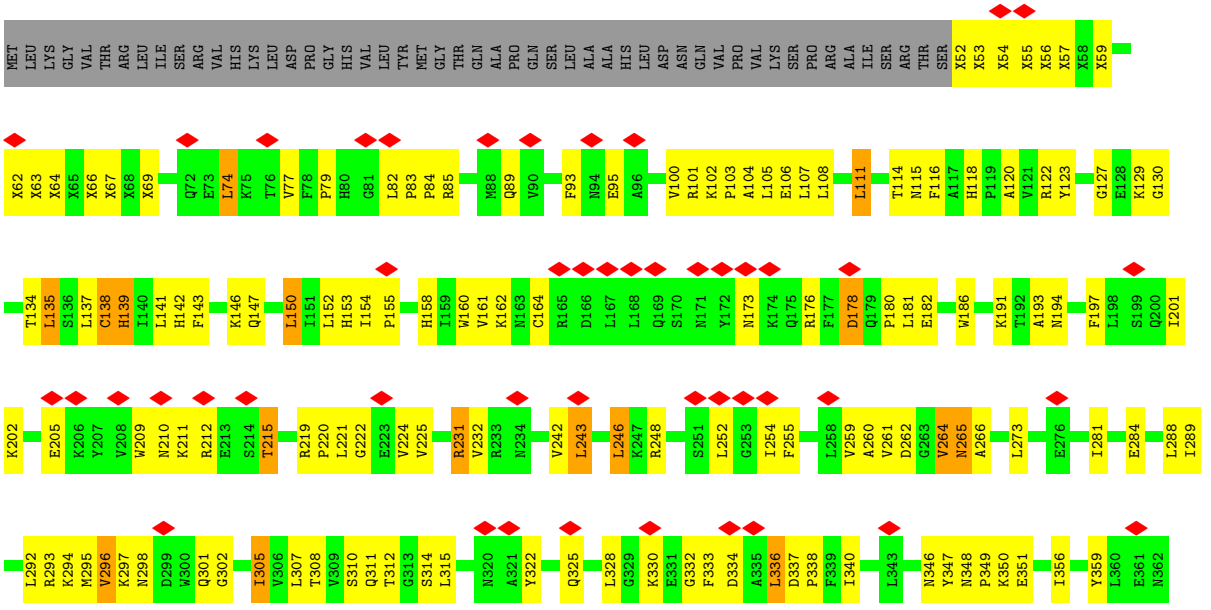
• Molecule 24: MITORIBOSOMAL PROTEIN MS28, MRPS28

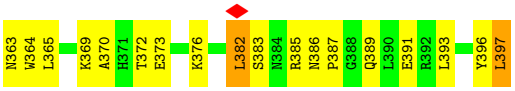
Chain Af:



• Molecule 25: MITORIBOSOMAL PROTEIN MS29, MRPS29

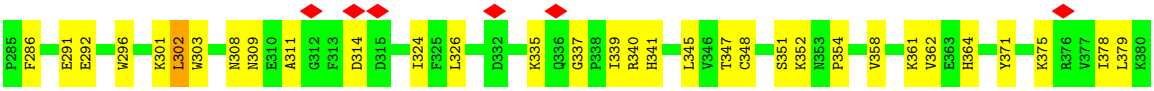
Chain Ag:

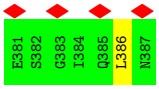




• Molecule 26: MITORIBOSOMAL PROTEIN MS31, MRPS31

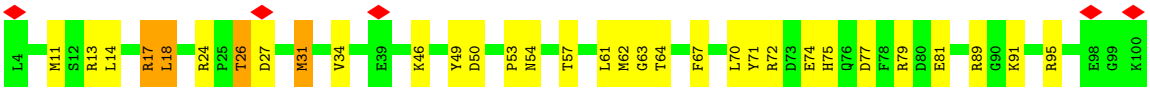
Chain Ah:





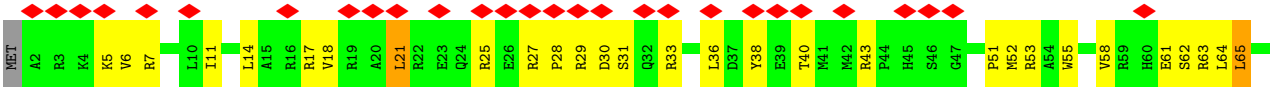
• Molecule 27: MITORIBOSOMAL PROTEIN MS33, MRPS33

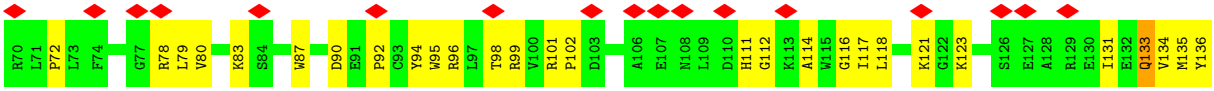
Chain Ai:

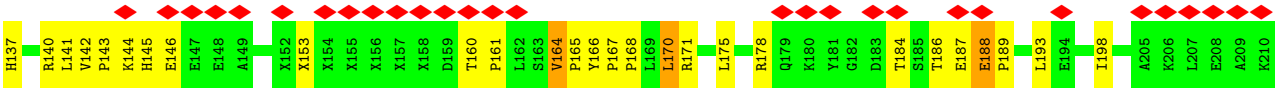


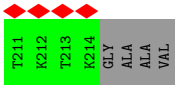
• Molecule 28: MITORIBOSOMAL PROTEIN MS34, MRPS34

Chain Aj:



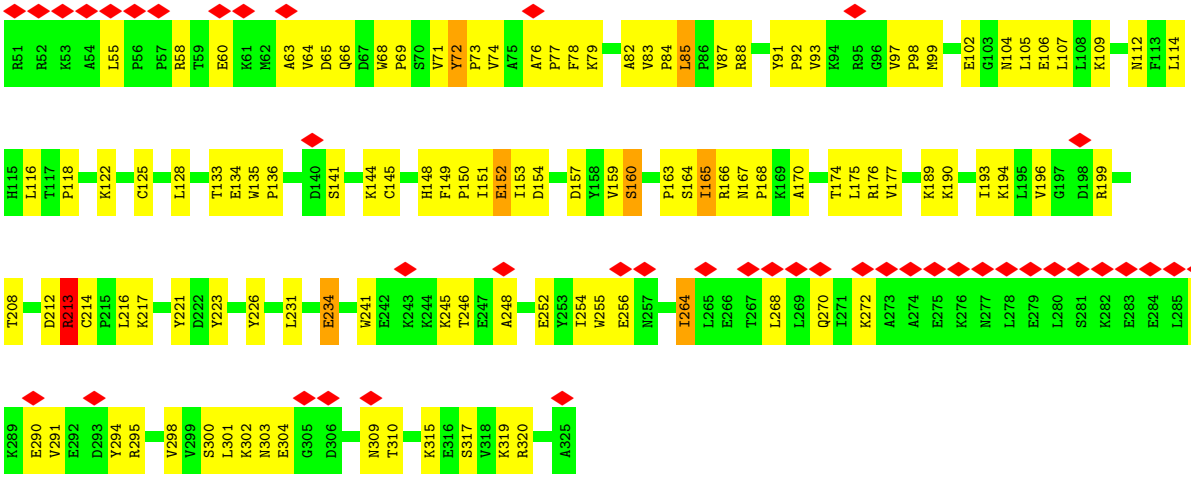




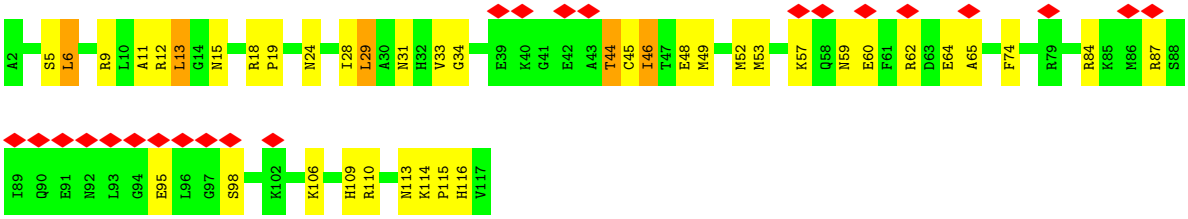


• Molecule 29: MITORIBOSOMAL PROTEIN MS35, MRPS35

Chain Ak:

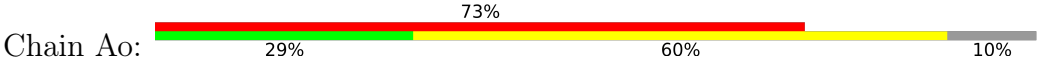


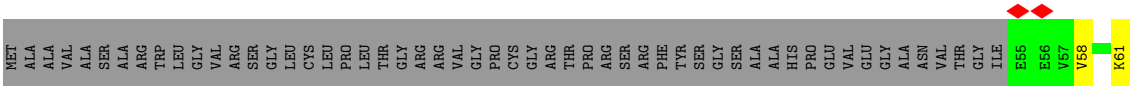
• Molecule 30: MITORIBOSOMAL PROTEIN MS37, MRPS37

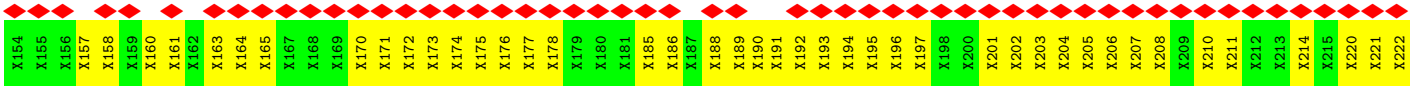


• Molecule 31: MITORIBOSOMAL PROTEIN MS38, MRPS38

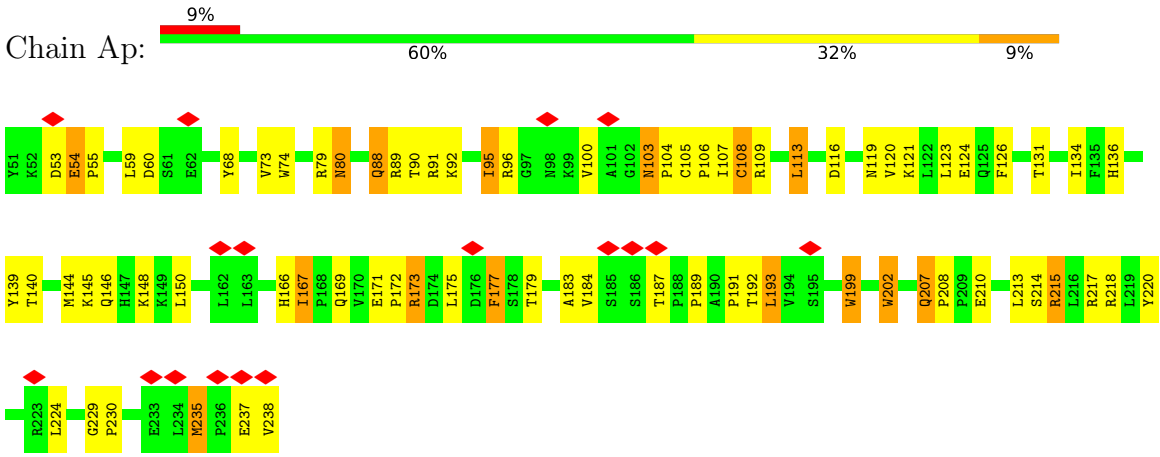
• Molecule 32: MITORIBOSOMAL PROTEIN MS39, MRPS39



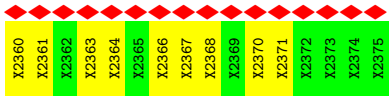




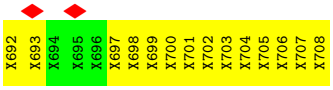
• Molecule 33: 28S RIBOSOMAL PROTEIN S18B, MITOCHONDRIAL



• Molecule 34: UNASSIGNED HELICES

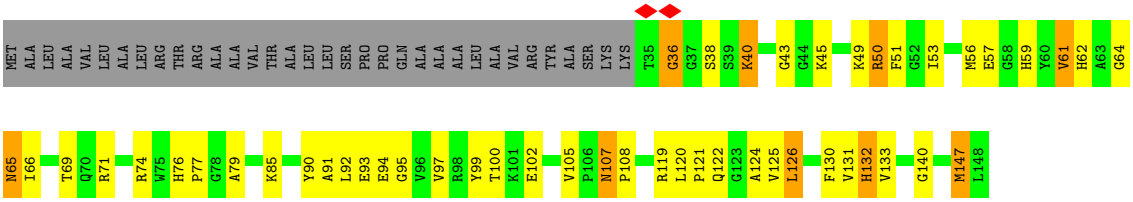


• Molecule 35: UNASSIGNED HELICES



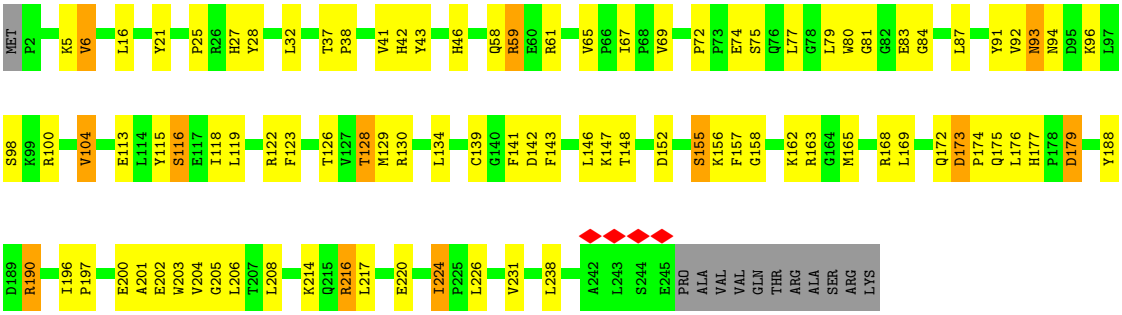
• Molecule 36: MITORIBOSOMAL PROTEIN BL27M, MRPL27

Chain B0:



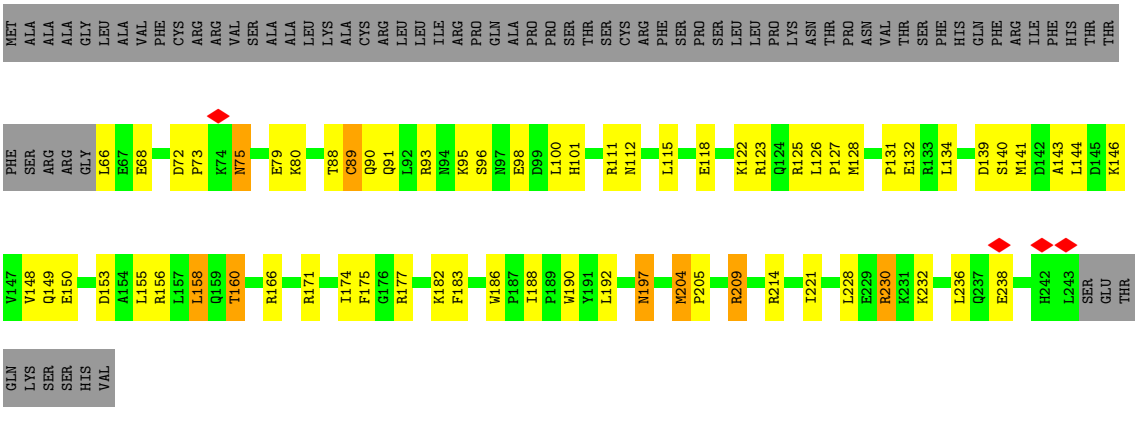
• Molecule 37: MITORIBOSOMAL PROTEIN BL28M, MRPL28

Chain B1:



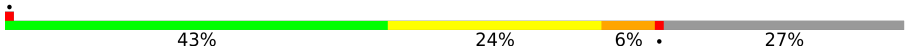
• Molecule 38: MITORIBOSOMAL PROTEIN UL29M, MRPL47

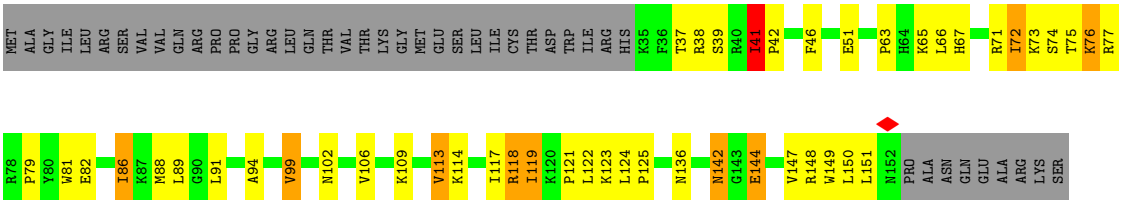
Chain B2:



• Molecule 39: MITORIBOSOMAL PROTEIN UL30M, MRPL30

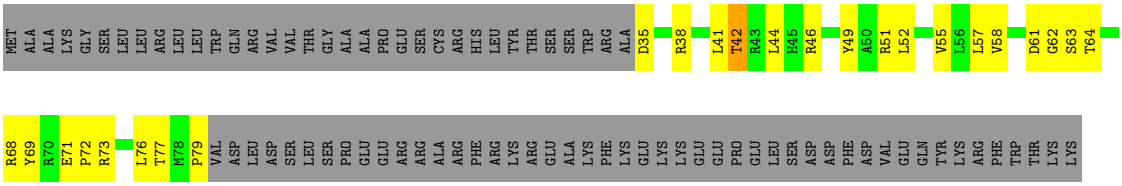
Chain B3:





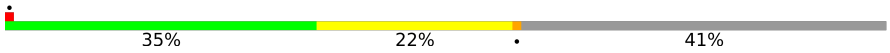
• Molecule 40: MITORIBOSOMAL PROTEIN BL31M, MRPL55

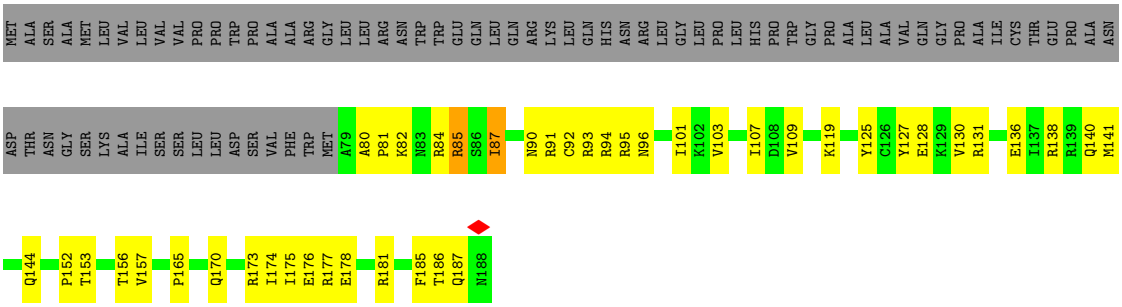
Chain B4:



• Molecule 41: MITORIBOSOMAL PROTEIN BL32M, MRPL32

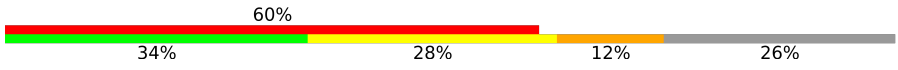
Chain B5:

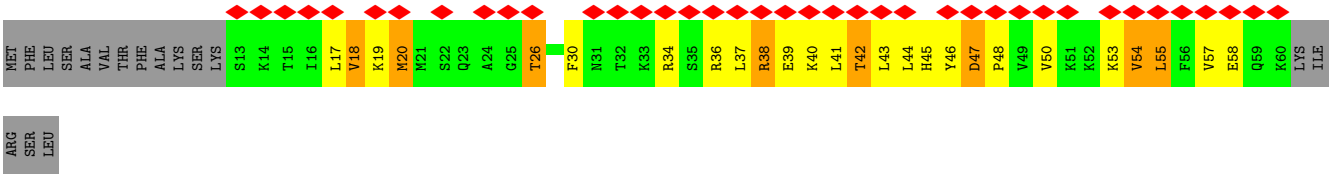




• Molecule 42: MITORIBOSOMAL PROTEIN BL33M, MRPL33

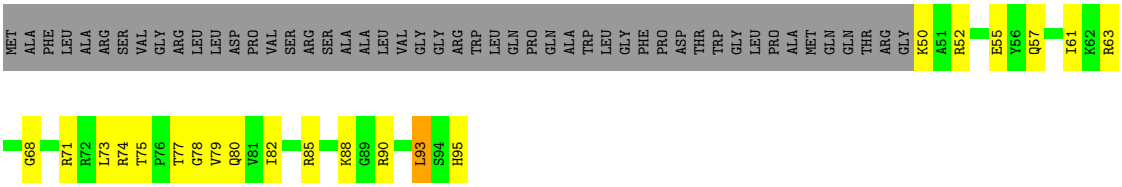
Chain B6:





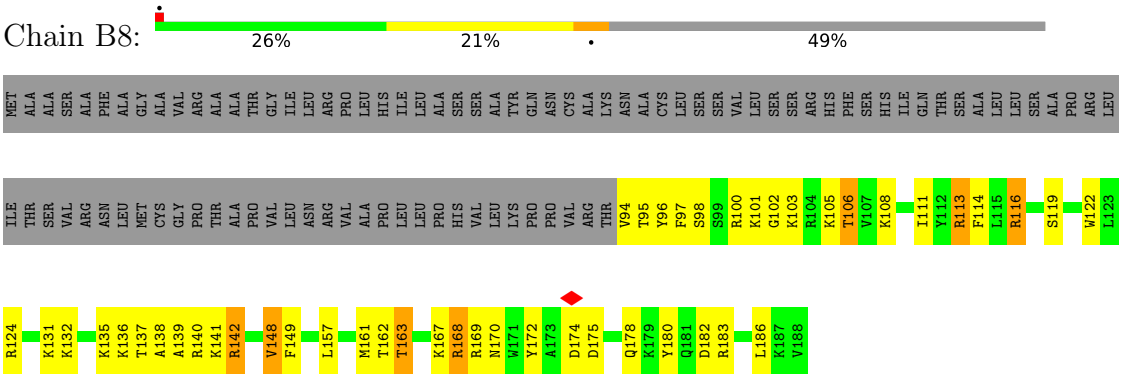
• Molecule 43: MITORIBOSOMAL PROTEIN BL34M, MRPL34

Chain B7:



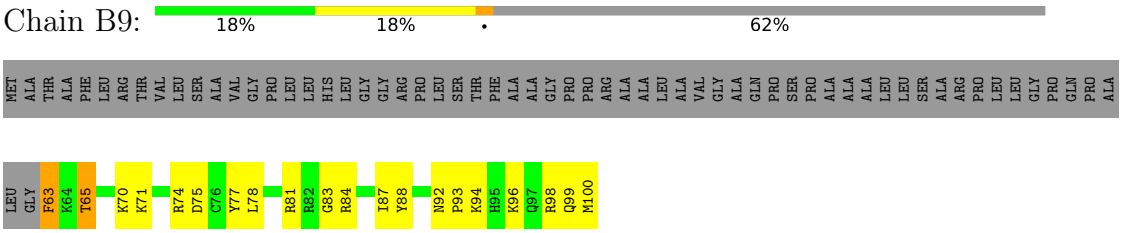
• Molecule 44: MITORIBOSOMAL PROTEIN BL35M, MRPL35

Chain B8:



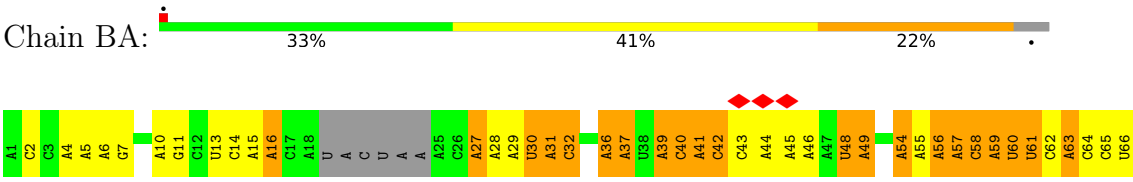
• Molecule 45: MITORIBOSOMAL PROTEIN BL36M, MRPL36

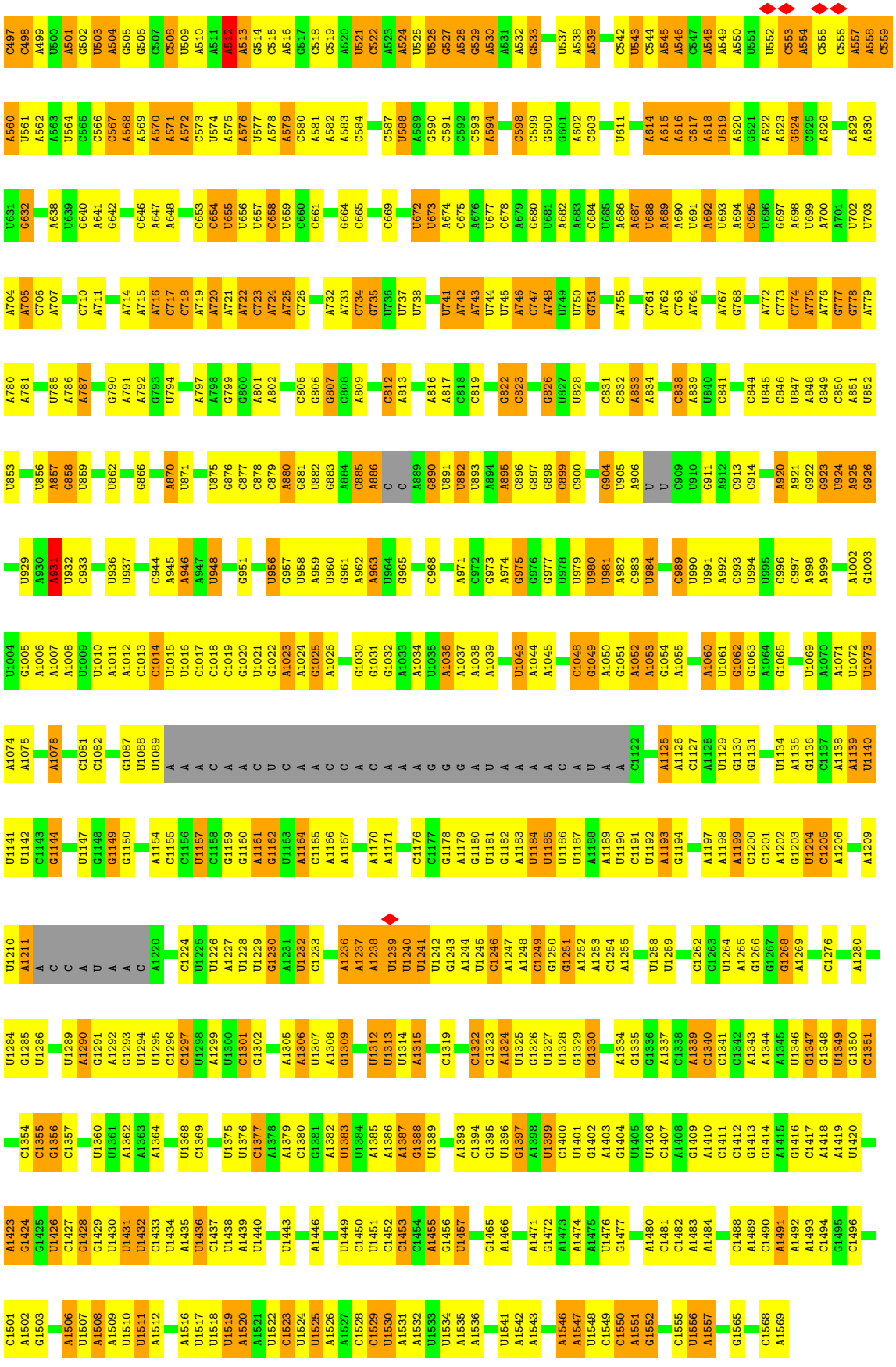
Chain B9:



• Molecule 46: MITORIBOSOMAL 16S Ribosomal RNA

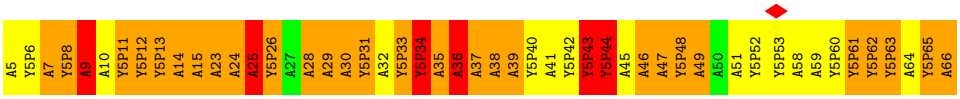
Chain BA:





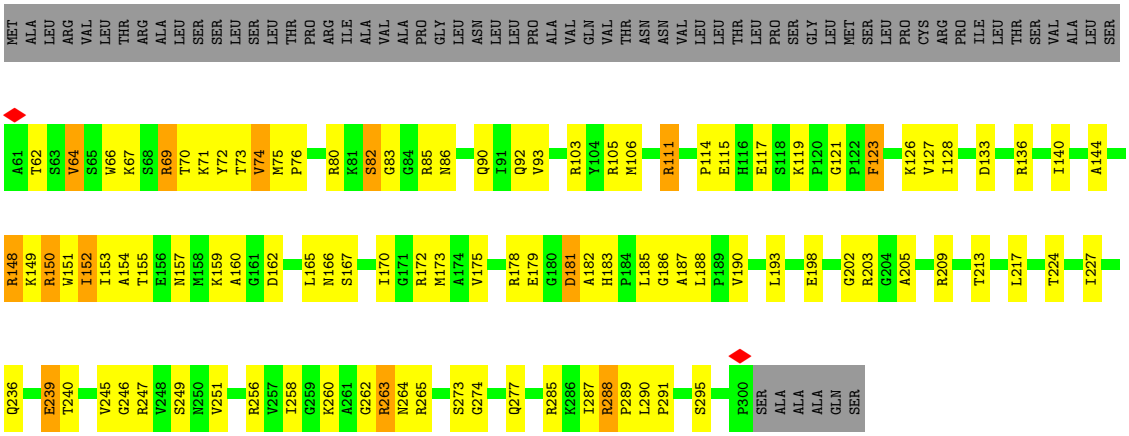
• Molecule 47: MITORIBOSOMAL CP TRNA

Chain BB:



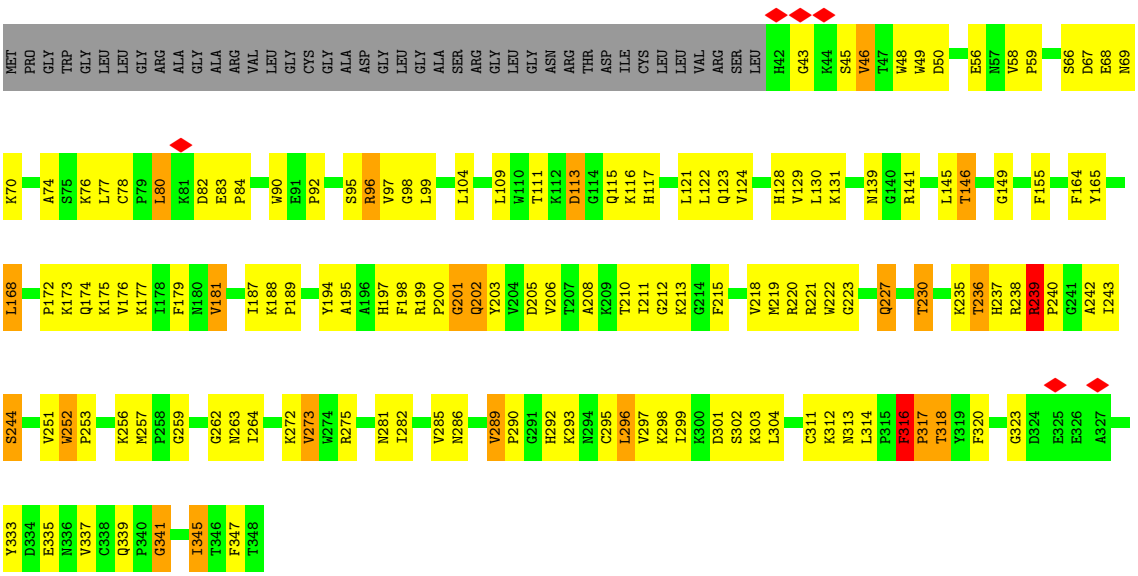
• Molecule 48: MITORIBOSOMAL PROTEIN UL2M, MRPL2

Chain BD:



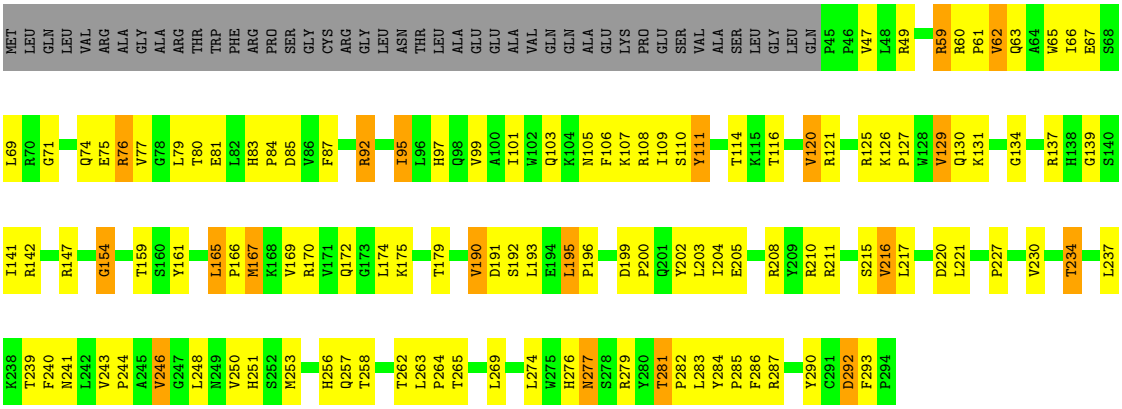
• Molecule 49: MITORIBOSOMAL PROTEIN UL3M, MRPL3

Chain BE:



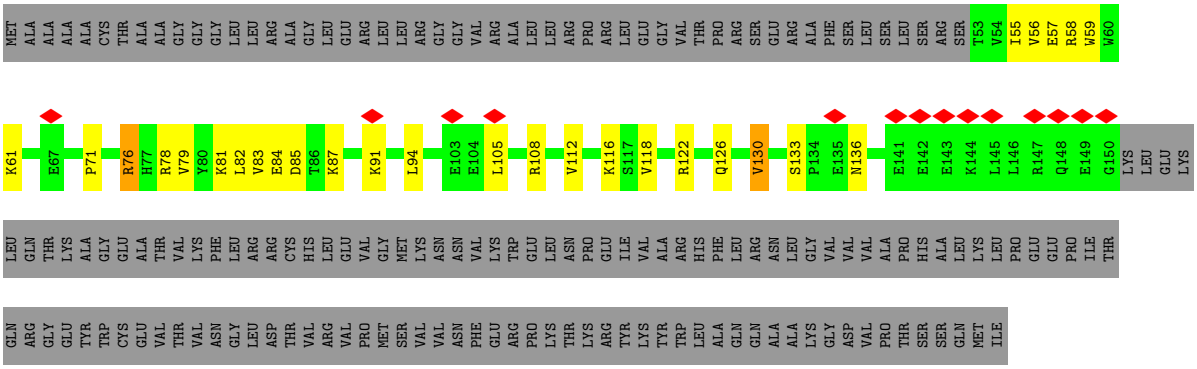
• Molecule 50: MITORIBOSOMAL PROTEIN UL4M, MRPL4

Chain BF:



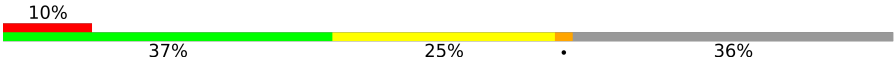
• Molecule 51: MITORIBOSOMAL PROTEIN BL9M, MRPL9

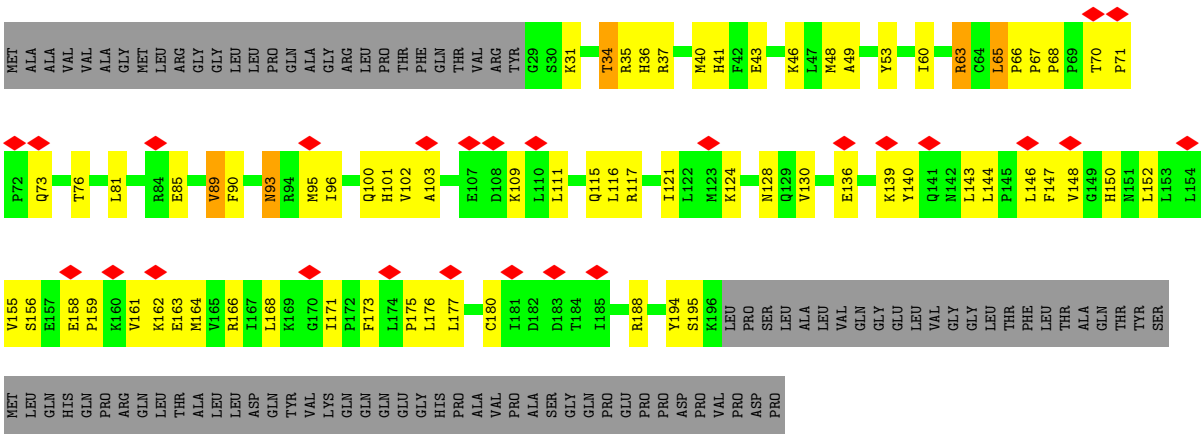
Chain BI:



• Molecule 52: MITORIBOSOMAL PROTEIN UL10M, MRPL10

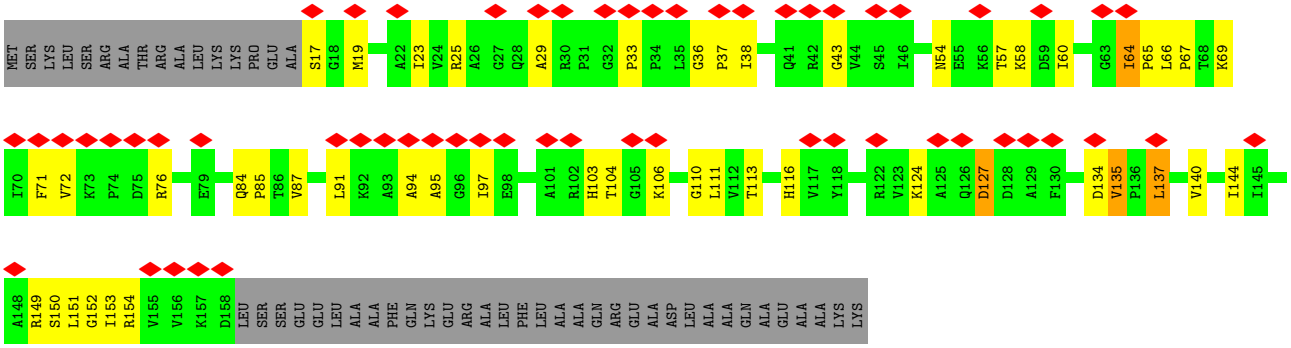
Chain BJ:





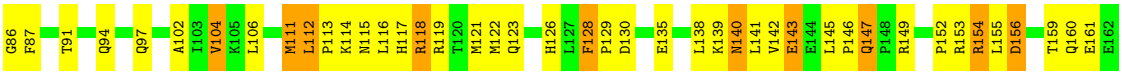
• Molecule 53: MITORIBOSOMAL PROTEIN UL11M, MRPL11

Chain BK:



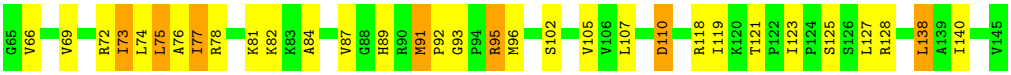
• Molecule 54: MITORIBOSOMAL PROTEIN UL13M, MRPL13

Chain BN:



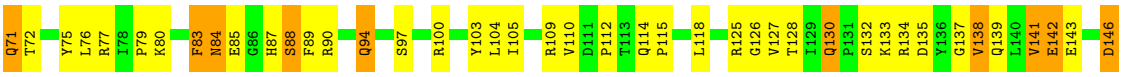
• Molecule 55: MITORIBOSOMAL PROTEIN UL14M, MRPL14

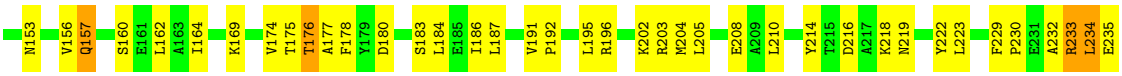
Chain BO:



• Molecule 56: MITORIBOSOMAL PROTEIN UL15M, MRPL15

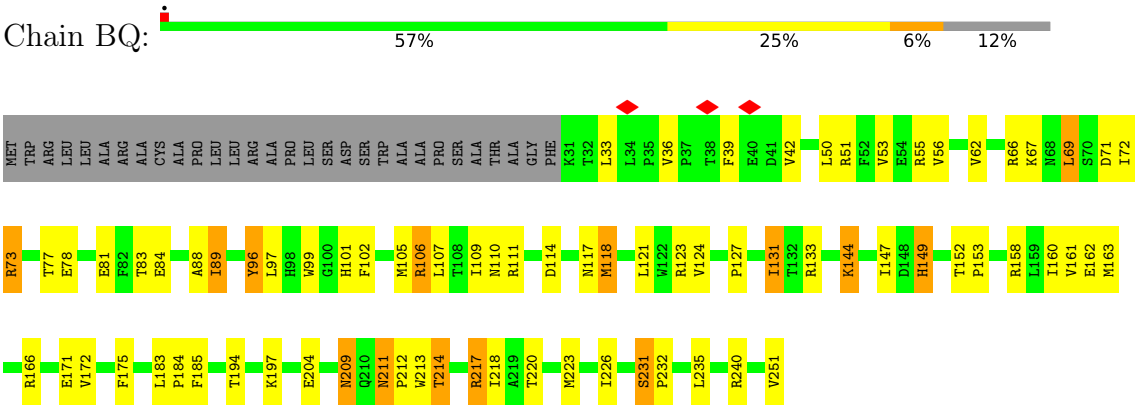
Chain BP:





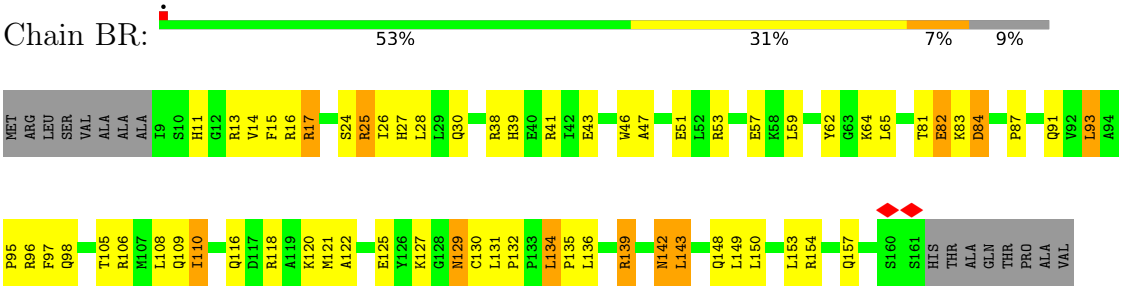
• Molecule 57: MITORIBOSOMAL PROTEIN UL16M, MRPL16

Chain BQ:



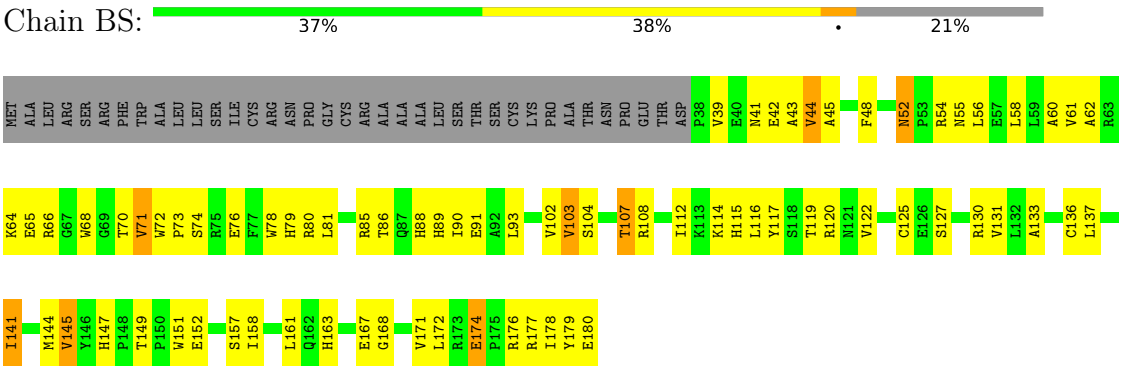
• Molecule 58: MITORIBOSOMAL PROTEIN BL17M, MRPL17

Chain BR:



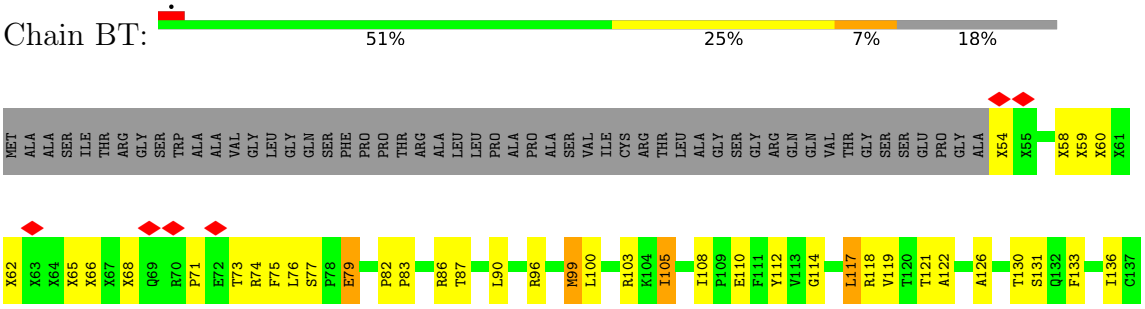
• Molecule 59: MITORIBOSOMAL PROTEIN UL18M, MRPL18

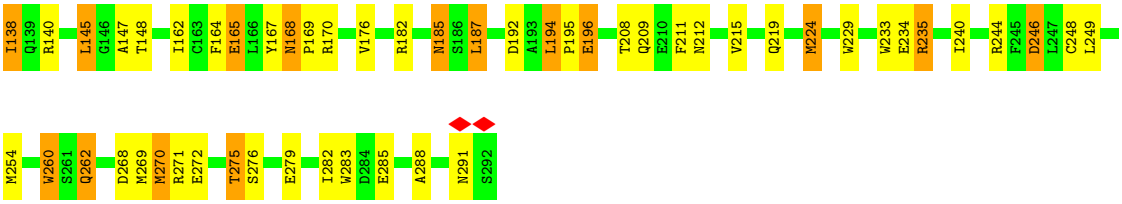
Chain BS:



• Molecule 60: MITORIBOSOMAL PROTEIN BL19M, MRPL19

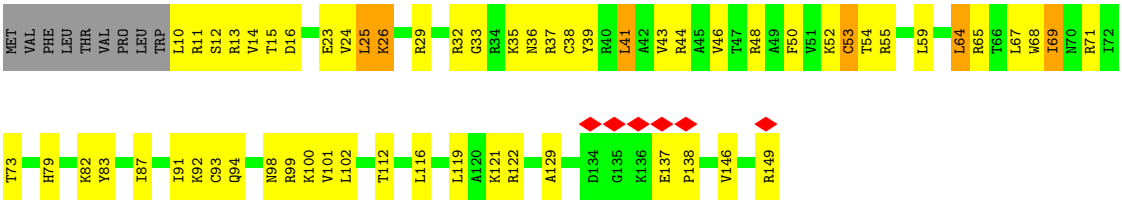
Chain BT:





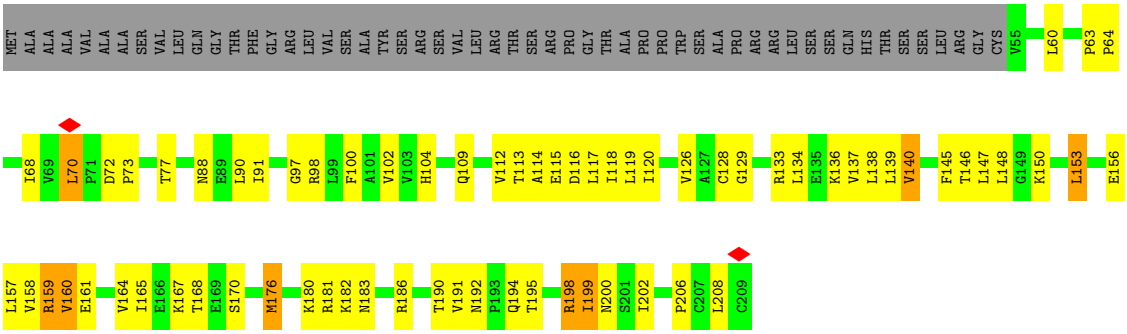
• Molecule 61: MITORIBOSOMAL PROTEIN BL20M, MRPL20

Chain BU:



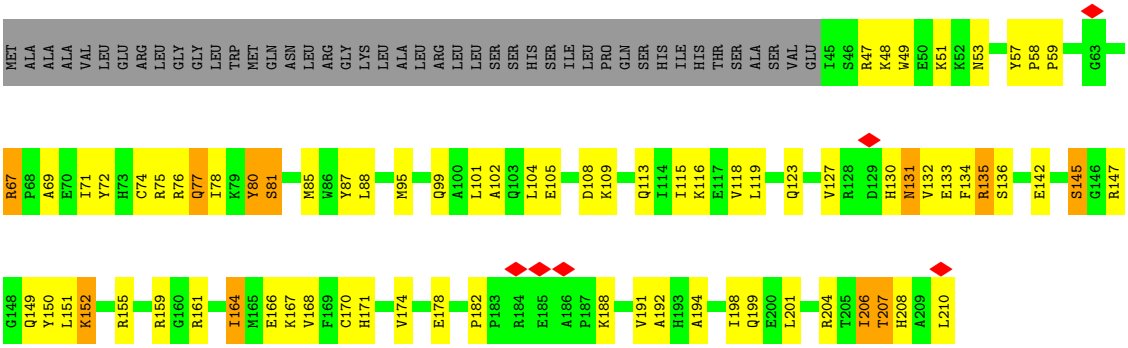
• Molecule 62: MITORIBOSOMAL PROTEIN BL21M, MRPL21

Chain BV:



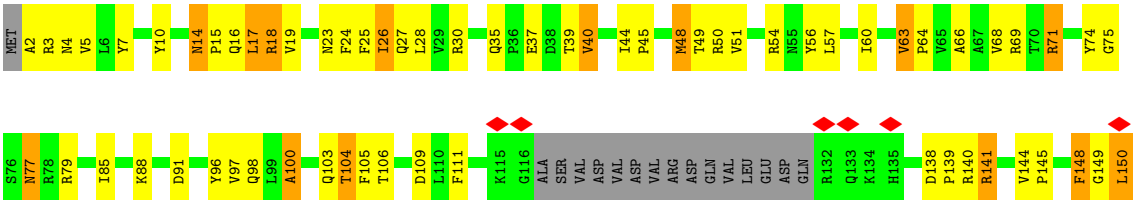
• Molecule 63: MITORIBOSOMAL PROTEIN UL22M, MRPL22

Chain BW:



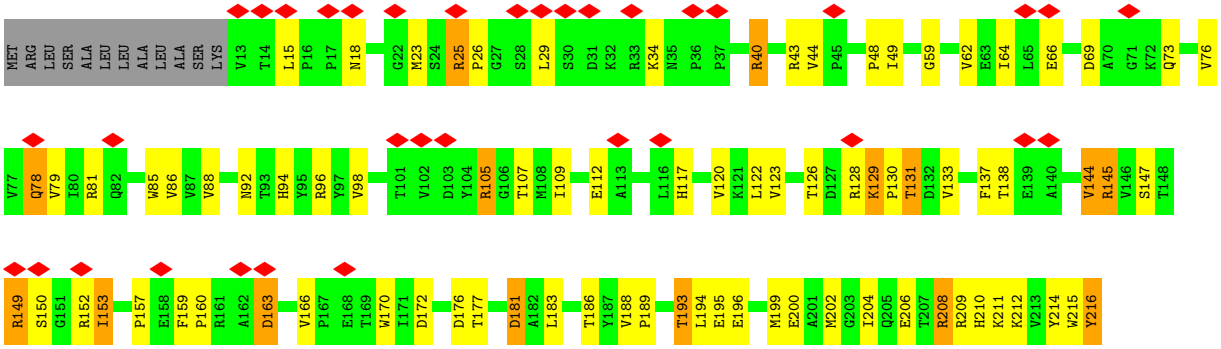
• Molecule 64: MITORIBOSOMAL PROTEIN UL23M, MRPL23

Chain BX:



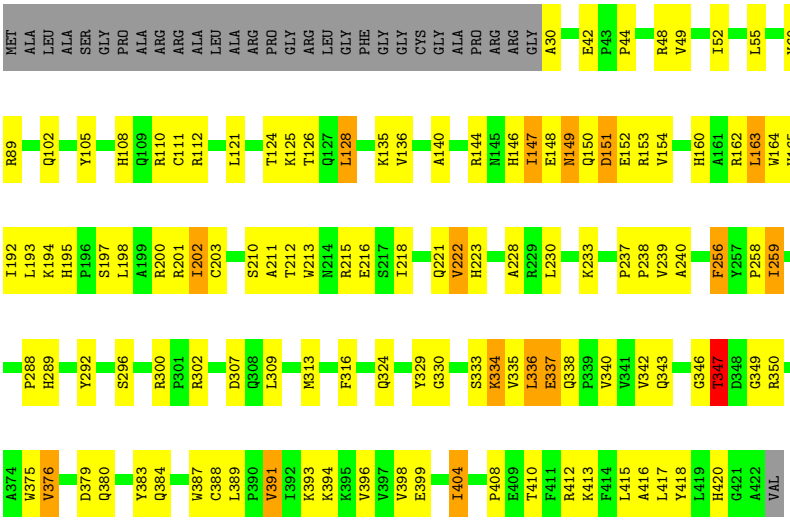
• Molecule 65: MITORIBOSOMAL PROTEIN UL24M, MRPL24

Chain BY:



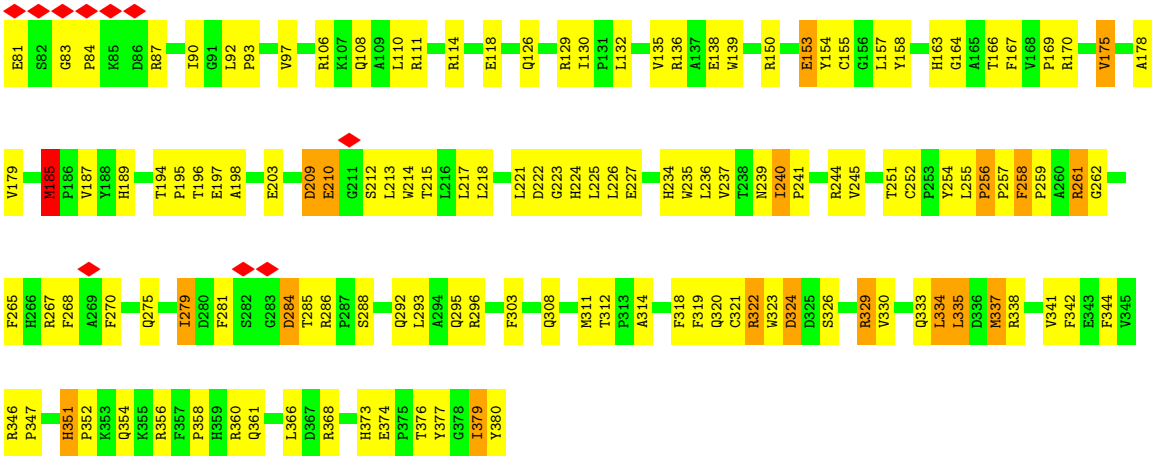
• Molecule 66: MITORIBOSOMAL PROTEIN ML37, MRPL37

Chain Ba:



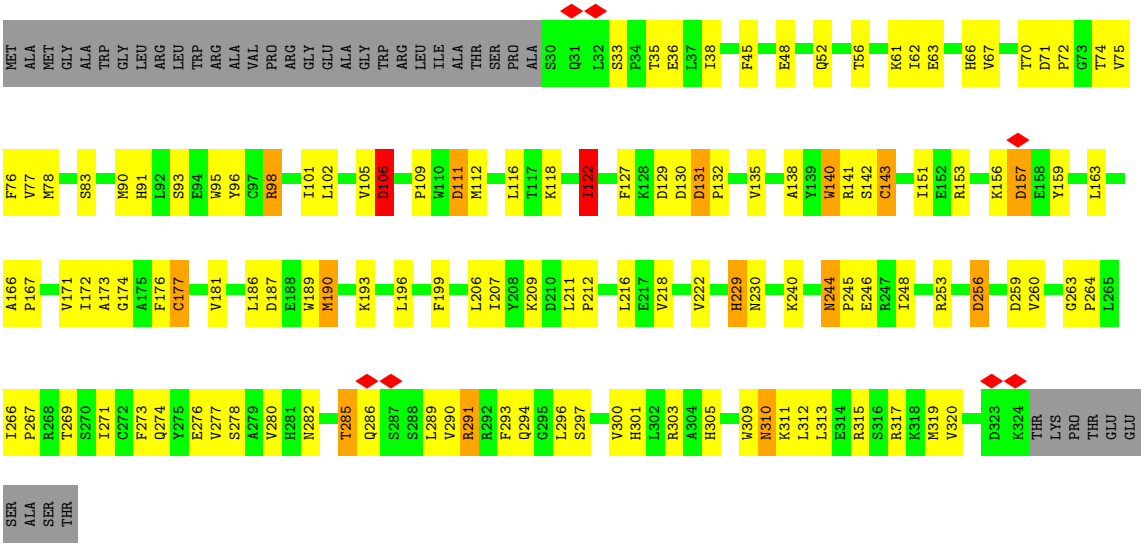
• Molecule 67: MITORIBOSOMAL PROTEIN ML38, MRPL38

Chain Bb:



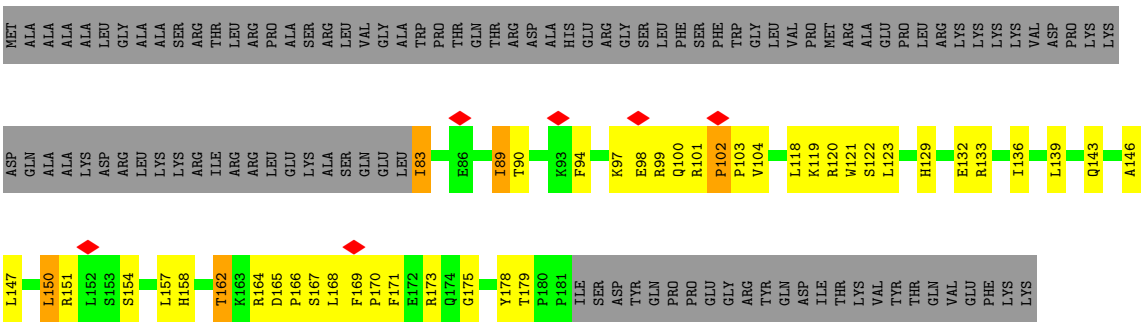
• Molecule 68: MITORIBOSOMAL PROTEIN ML39, MRPL39

Chain Bc:



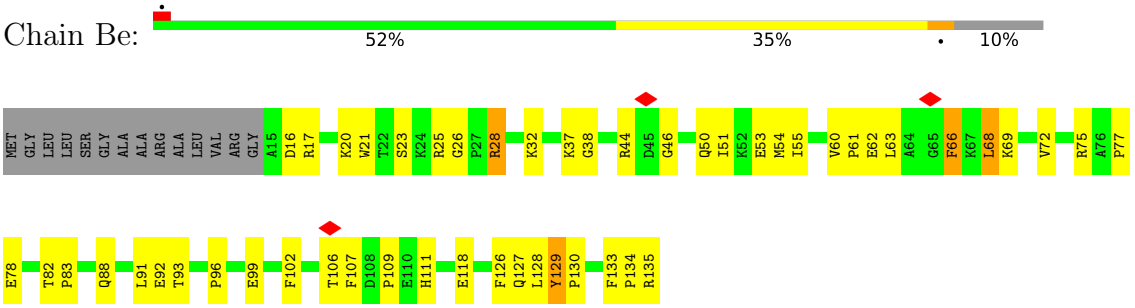
• Molecule 69: MITORIBOSOMAL PROTEIN ML40, MRPL40

Chain Bd:



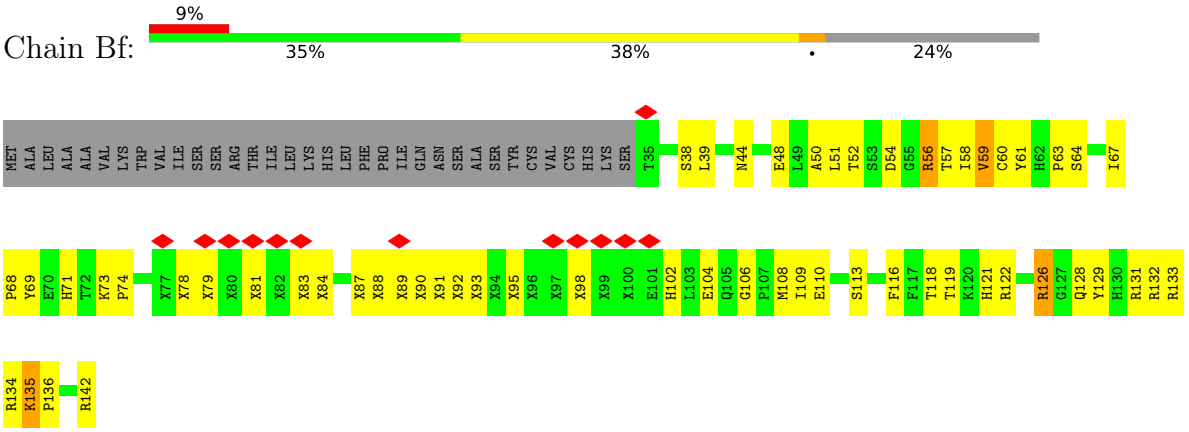
• Molecule 70: MITORIBOSOMAL PROTEIN ML41, MRPL41

Chain Be:



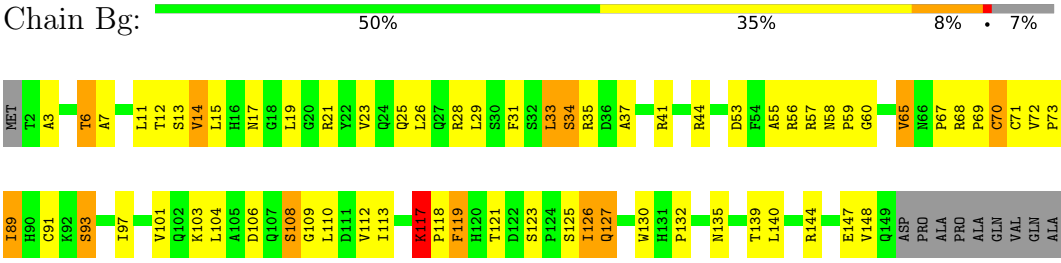
• Molecule 71: MITORIBOSOMAL PROTEIN ML42, MRPL42

Chain Bf:



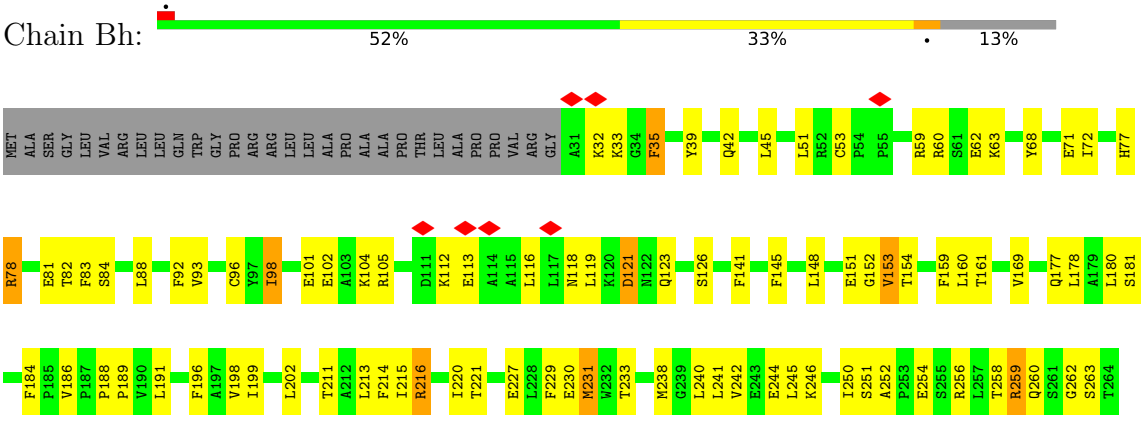
• Molecule 72: MITORIBOSOMAL PROTEIN ML43, MRPL43

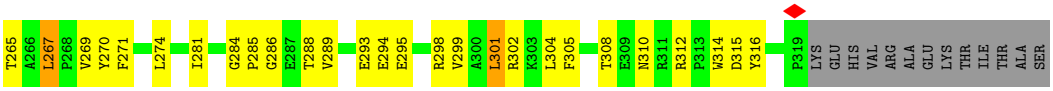
Chain Bg:



• Molecule 73: MITORIBOSOMAL PROTEIN ML44, MRPL44

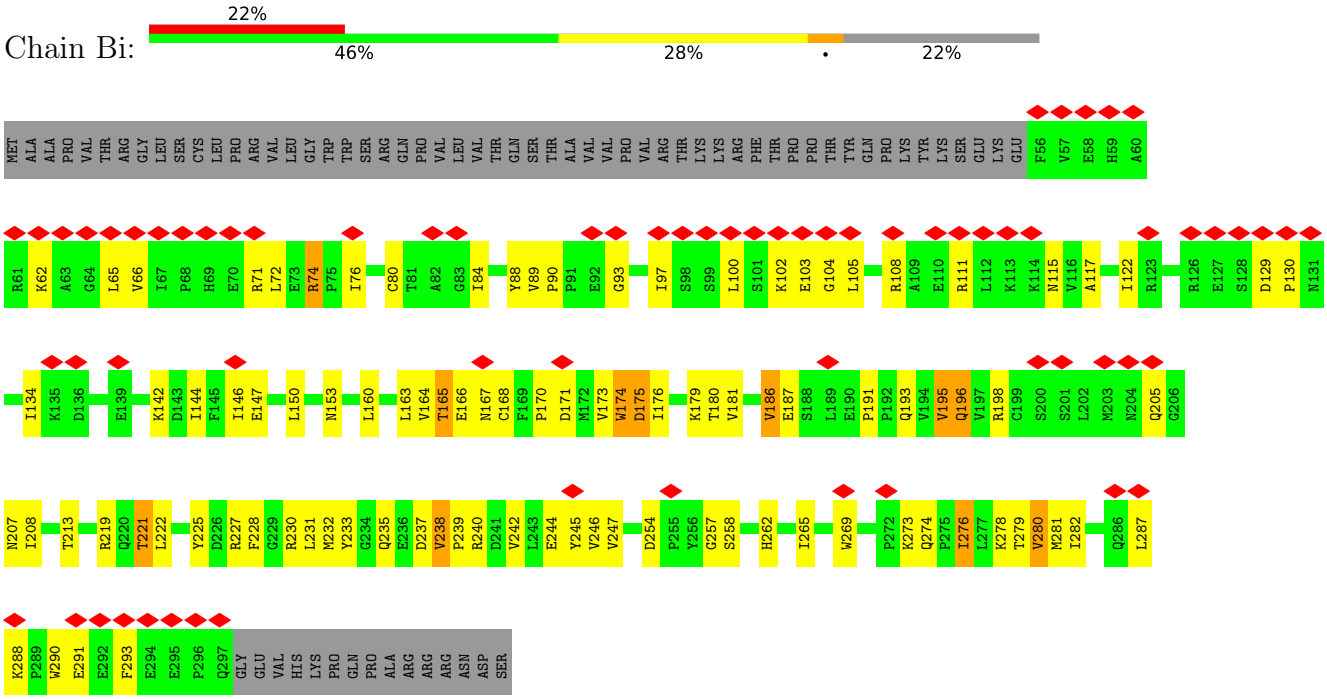
Chain Bh:





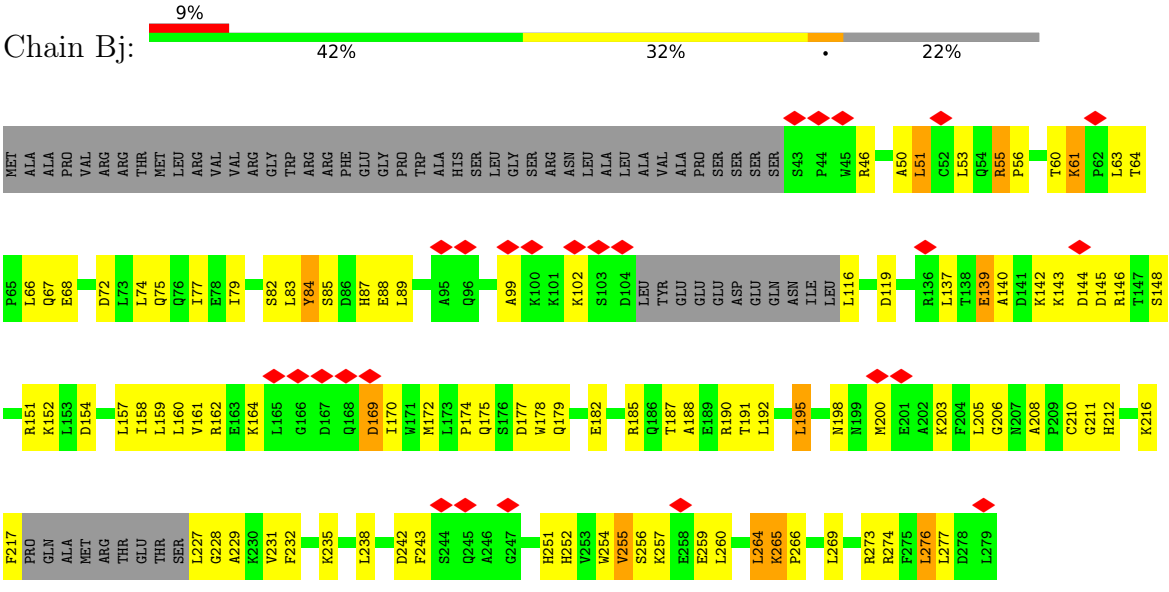
• Molecule 74: MITORIBOSOMAL PROTEIN ML45, MRPL45

Chain Bi:



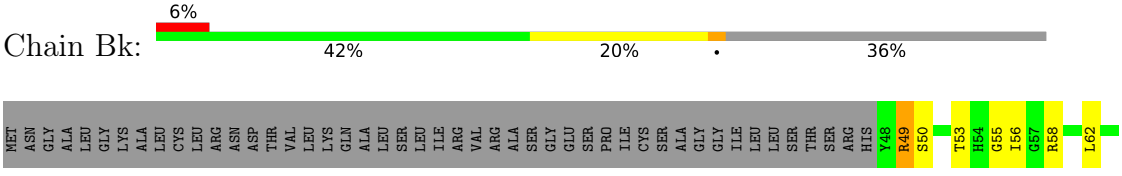
• Molecule 75: MITORIBOSOMAL PROTEIN ML46, MRPL46

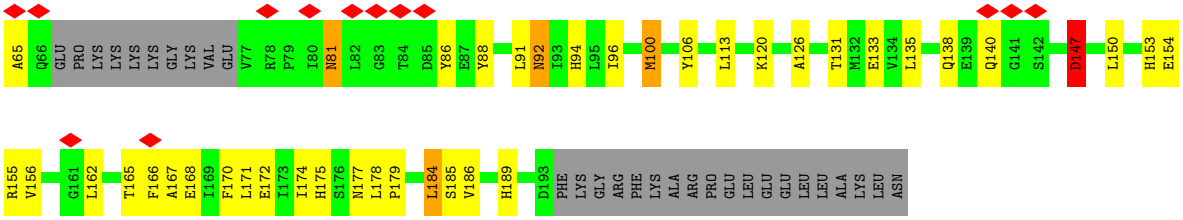
Chain Bj:



• Molecule 76: MITORIBOSOMAL PROTEIN ML48, MRPL48

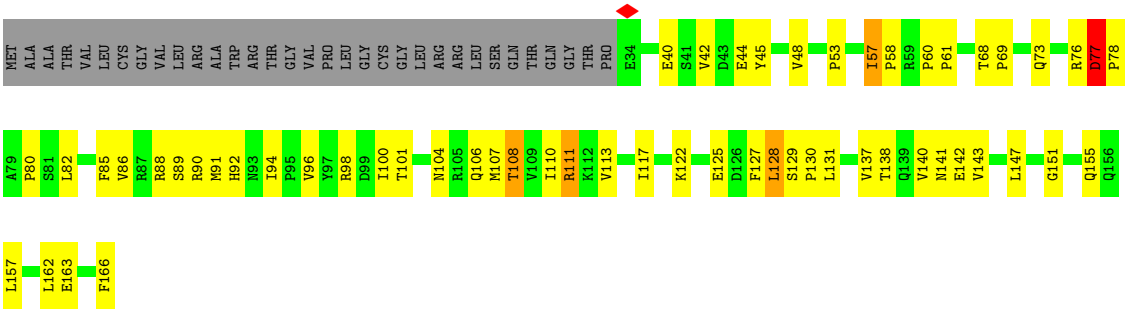
Chain Bk:





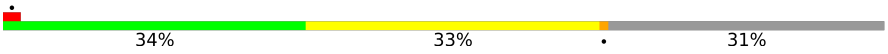
• Molecule 77: MITORIBOSOMAL PROTEIN ML49, MRPL49

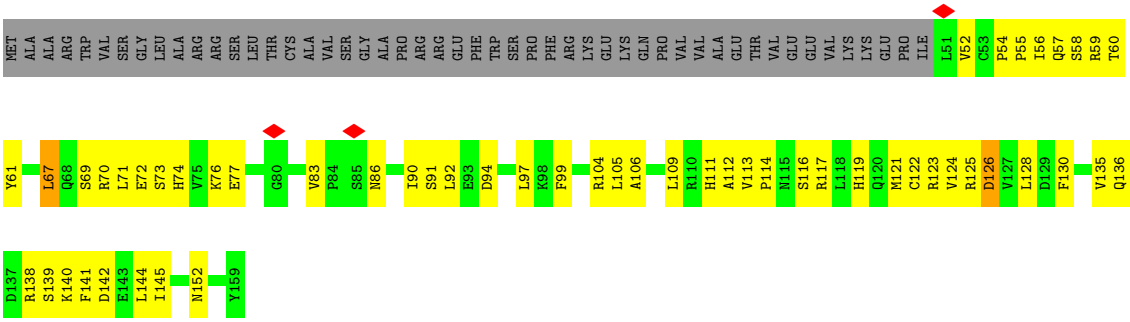
Chain Bl:



• Molecule 78: MITORIBOSOMAL PROTEIN ML50, MRPL50

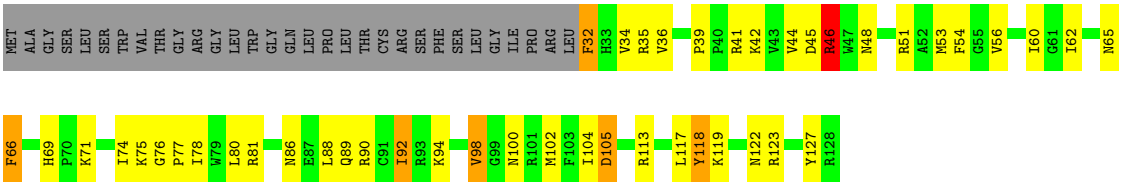
Chain Bm:





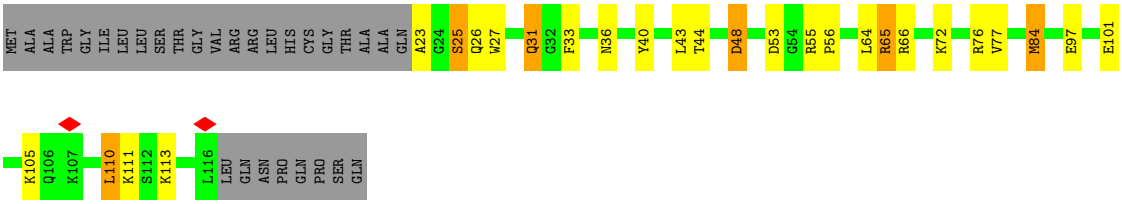
• Molecule 79: MITORIBOSOMAL PROTEIN ML51, MRPL51

Chain Bn:



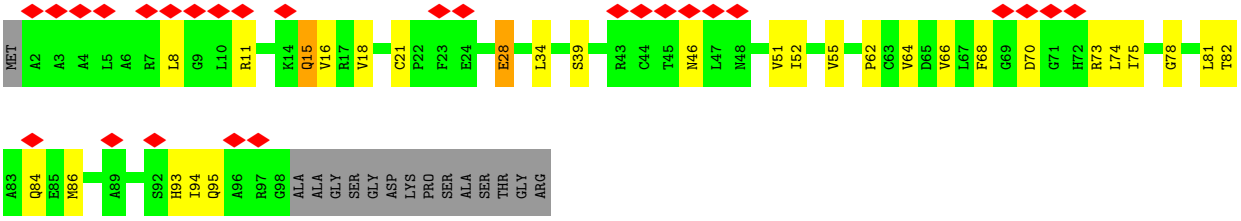
• Molecule 80: MITORIBOSOMAL PROTEIN ML52, MRPL52

Chain Bo:



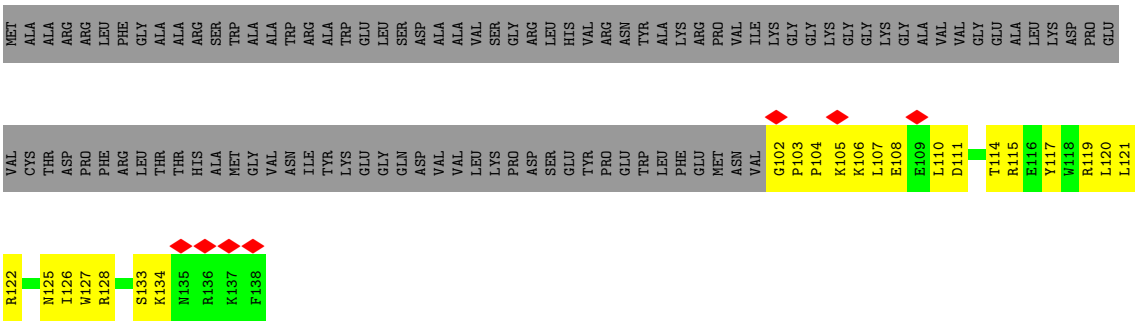
• Molecule 81: MITORIBOSOMAL PROTEIN ML53, MRPL53

Chain Bp:



• Molecule 82: MITORIBOSOMAL PROTEIN ML54, MRPL54

Chain Bq:

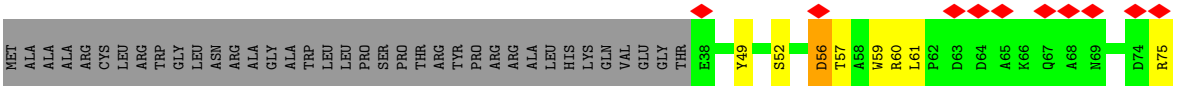


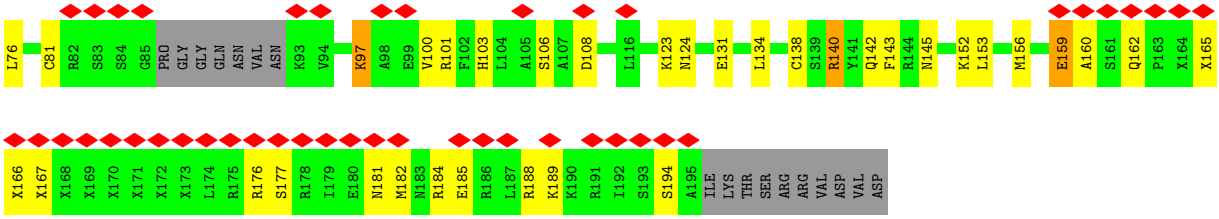
• Molecule 83: MITORIBOSOMAL PROTEIN ML63, MRPL57

Chain Bt:

• Molecule 84: MITORIBOSOMAL PROTEIN ML62, MRPL58

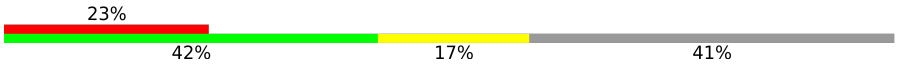
Chain Bu:

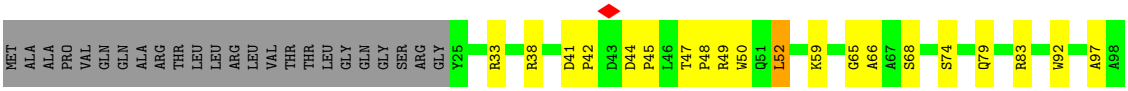


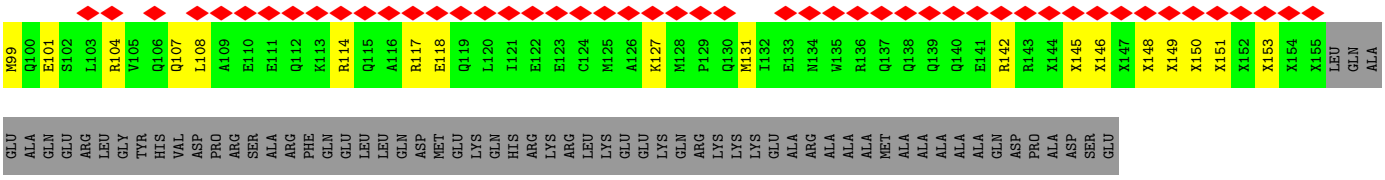


• Molecule 85: MITORIBOSOMAL PROTEIN ML64, MRPL59

Chain Bv:

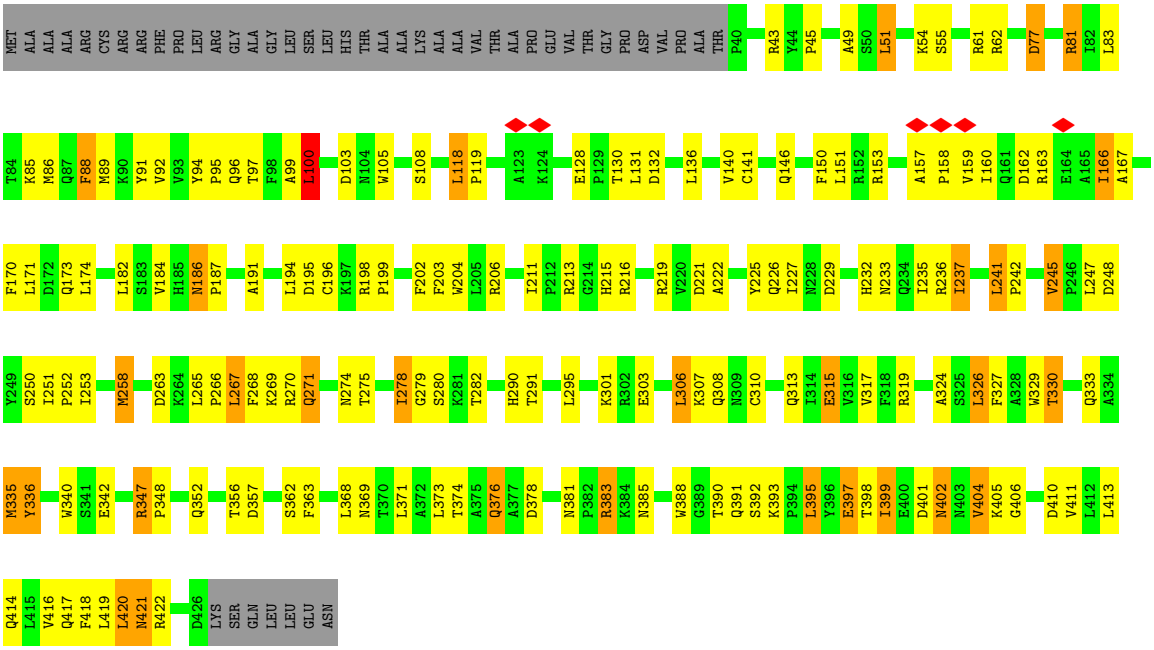






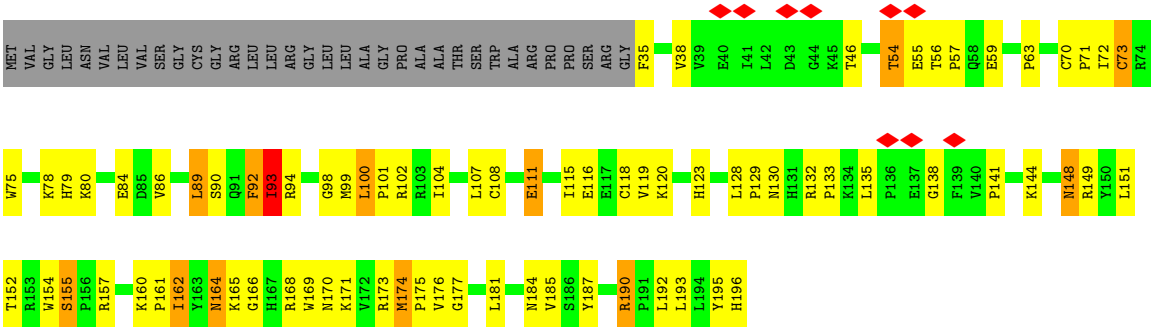
• Molecule 86: MITORIBOSOMAL PROTEIN ML65, MRPS30

Chain Bw:



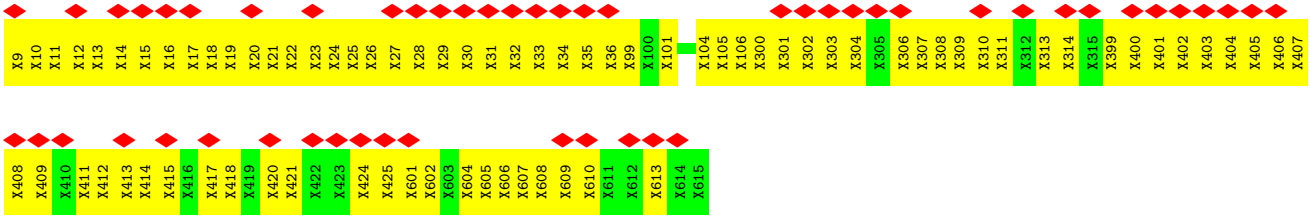
• Molecule 87: MITORIBOSOMAL PROTEIN ML66, MRPS18A

Chain Bx:



• Molecule 88: UNASSIGNED SECONDARY STRUCTURE ELEMENTS

Chain Bz:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	60872	Depositor
Resolution determination method	Not provided	
CTF correction method	PER DETECTOR FRAME	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	100000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.391	Depositor
Minimum map value	-0.186	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	355.84, 355.84, 355.84	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: Y5P, ZN, MG, GDP, P5P

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	AA	0.25	0/22852	0.41	0/35580
2	AB	0.47	0/1804	0.88	5/2445 (0.2%)
3	AC	0.44	0/1105	0.93	5/1496 (0.3%)
4	AE	0.43	0/2673	0.84	2/3591 (0.1%)
5	AF	0.48	0/1008	0.99	5/1358 (0.4%)
6	AG	0.46	0/1763	0.85	4/2368 (0.2%)
7	AI	0.44	1/2455 (0.0%)	0.82	5/3291 (0.2%)
8	AJ	0.47	0/1091	0.93	2/1474 (0.1%)
9	AK	0.51	0/1021	1.01	3/1381 (0.2%)
10	AL	0.42	0/858	0.97	5/1152 (0.4%)
11	AN	0.40	0/874	0.79	0/1171
12	AO	0.47	0/1473	0.93	6/1970 (0.3%)
13	AP	0.47	0/954	0.86	5/1284 (0.4%)
14	AQ	0.46	0/871	1.01	3/1181 (0.3%)
15	AR	0.51	0/802	0.93	5/1079 (0.5%)
16	AU	0.46	0/745	0.88	2/993 (0.2%)
19	Aa	0.46	0/2052	0.76	0/2774
20	Ab	0.42	0/1126	0.88	2/1514 (0.1%)
21	Ac	0.42	0/1399	0.94	4/1881 (0.2%)
22	Ad	0.46	0/1490	0.80	2/2005 (0.1%)
24	Af	0.38	0/790	0.86	2/1064 (0.2%)
25	Ag	0.47	0/2731	0.83	0/3696
26	Ah	0.38	0/903	0.85	3/1215 (0.2%)
27	Ai	0.39	0/841	0.81	0/1121
28	Aj	0.44	0/1779	0.91	7/2404 (0.3%)
29	Ak	0.44	0/2268	0.91	3/3069 (0.1%)
30	Am	0.48	0/947	0.90	2/1268 (0.2%)
31	An	0.53	0/650	0.90	2/858 (0.2%)
32	Ao	0.43	0/726	0.95	4/988 (0.4%)
33	Ap	0.46	0/1602	1.00	11/2175 (0.5%)
36	B0	0.70	0/901	1.10	7/1217 (0.6%)
37	B1	0.49	0/2093	0.88	3/2835 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	B2	0.52	0/1582	0.87	0/2118
39	B3	0.61	0/993	1.15	8/1341 (0.6%)
40	B4	0.37	0/388	1.08	3/523 (0.6%)
41	B5	0.56	0/917	0.96	5/1227 (0.4%)
42	B6	0.47	0/396	1.05	2/526 (0.4%)
43	B7	0.80	0/395	0.98	2/524 (0.4%)
44	B8	0.69	0/853	1.00	3/1136 (0.3%)
45	B9	0.70	0/342	0.87	0/450
46	BA	0.42	0/36094	0.56	4/56186 (0.0%)
48	BD	0.65	0/1898	1.06	10/2555 (0.4%)
49	BE	0.61	0/2493	1.09	17/3387 (0.5%)
50	BF	0.67	1/2069 (0.0%)	1.01	5/2816 (0.2%)
51	BI	0.50	0/819	0.87	0/1101
52	BJ	0.53	0/1392	1.01	8/1881 (0.4%)
53	BK	0.52	0/1099	0.92	4/1480 (0.3%)
54	BN	0.65	0/1487	1.05	11/2017 (0.5%)
55	BO	0.64	1/912 (0.1%)	0.97	1/1231 (0.1%)
56	BP	0.58	0/2368	1.03	8/3198 (0.3%)
57	BQ	0.60	0/1838	0.97	3/2475 (0.1%)
58	BR	0.59	0/1262	0.89	2/1700 (0.1%)
59	BS	0.52	0/1197	0.93	1/1624 (0.1%)
60	BT	0.55	0/1903	1.01	8/2567 (0.3%)
61	BU	0.72	0/1179	0.94	0/1578
62	BV	0.65	0/1256	1.01	2/1706 (0.1%)
63	BW	0.63	0/1407	0.95	2/1891 (0.1%)
64	BX	0.52	0/1149	1.05	5/1554 (0.3%)
65	BY	0.47	0/1704	0.96	6/2310 (0.3%)
66	Ba	0.52	0/3267	0.94	7/4455 (0.2%)
67	Bb	0.49	0/3047	0.97	10/4139 (0.2%)
68	Bc	0.45	0/2464	0.90	9/3330 (0.3%)
69	Bd	0.48	0/853	0.99	7/1153 (0.6%)
70	Be	0.52	0/996	1.01	5/1340 (0.4%)
71	Bf	0.51	0/731	1.00	2/990 (0.2%)
72	Bg	0.60	0/1191	1.08	8/1614 (0.5%)
73	Bh	0.52	0/2372	0.97	4/3211 (0.1%)
74	Bi	0.50	0/2034	0.90	5/2759 (0.2%)
75	Bj	0.43	0/1811	0.89	6/2436 (0.2%)
76	Bk	0.50	0/1108	0.96	1/1499 (0.1%)
77	Bl	0.56	0/1135	0.99	2/1549 (0.1%)
78	Bm	0.45	0/917	0.86	0/1248
79	Bn	0.71	0/860	1.06	4/1150 (0.3%)
80	Bo	0.57	0/762	0.93	1/1022 (0.1%)
81	Bp	0.49	0/752	0.95	3/1013 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
82	Bq	0.42	0/346	0.76	2/463 (0.4%)
83	Bt	0.63	0/798	1.20	5/1073 (0.5%)
84	Bu	0.45	0/1163	0.81	2/1557 (0.1%)
85	Bv	0.49	0/1022	0.78	1/1382 (0.1%)
86	Bw	0.57	0/3206	0.99	9/4354 (0.2%)
87	Bx	0.55	0/1364	1.04	7/1849 (0.4%)
All	All	0.47	3/166238 (0.0%)	0.80	329/236586 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
9	AK	0	1
49	BE	0	1
57	BQ	0	1
60	BT	0	1
67	Bb	0	2
79	Bn	0	1
83	Bt	0	1
All	All	0	8

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	BO	58	ILE	CA-CB	-6.02	1.49	1.55
7	AI	249	ILE	CA-C	5.87	1.56	1.52
50	BF	141	ILE	CA-CB	-5.48	1.47	1.54

All (329) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
83	Bt	23	ARG	CA-C-N	12.01	131.59	119.82
83	Bt	23	ARG	C-N-CA	12.01	131.59	119.82
73	Bh	284	GLY	CA-C-N	11.44	131.52	120.31
73	Bh	284	GLY	C-N-CA	11.44	131.52	120.31
12	AO	68	PRO	CA-C-N	10.22	130.91	120.38
12	AO	68	PRO	C-N-CA	10.22	130.91	120.38
52	BJ	70	THR	CA-C-N	9.97	130.65	120.38
52	BJ	70	THR	C-N-CA	9.97	130.65	120.38
72	Bg	117	LYS	CA-C-N	9.77	129.39	119.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
72	Bg	117	LYS	C-N-CA	9.77	129.39	119.82
33	Ap	230	PRO	CA-C-N	9.68	130.35	120.38
33	Ap	230	PRO	C-N-CA	9.68	130.35	120.38
83	Bt	25	ARG	CA-C-N	9.29	129.41	120.31
83	Bt	25	ARG	C-N-CA	9.29	129.41	120.31
42	B6	47	ASP	CA-C-N	9.17	128.84	118.85
42	B6	47	ASP	C-N-CA	9.17	128.84	118.85
64	BX	111	PHE	CA-C-N	9.16	129.39	119.87
64	BX	111	PHE	C-N-CA	9.16	129.39	119.87
29	Ak	76	ALA	CA-C-N	8.98	128.62	119.82
29	Ak	76	ALA	C-N-CA	8.98	128.62	119.82
14	AQ	36	ASP	CA-C-N	8.87	129.04	119.28
14	AQ	36	ASP	C-N-CA	8.87	129.04	119.28
28	Aj	164	VAL	CA-C-N	8.41	130.35	119.84
28	Aj	164	VAL	C-N-CA	8.41	130.35	119.84
7	AI	249	ILE	N-CA-C	8.38	117.58	107.61
65	BY	15	LEU	CA-C-N	8.31	128.94	120.38
65	BY	15	LEU	C-N-CA	8.31	128.94	120.38
33	Ap	54	GLU	CA-C-N	8.21	127.79	118.85
33	Ap	54	GLU	C-N-CA	8.21	127.79	118.85
73	Bh	35	PHE	N-CA-C	-8.11	102.42	111.82
86	Bw	381	ASN	CA-C-N	8.00	127.57	118.85
86	Bw	381	ASN	C-N-CA	8.00	127.57	118.85
36	B0	105	VAL	CA-C-N	7.90	128.38	119.92
36	B0	105	VAL	C-N-CA	7.90	128.38	119.92
48	BD	119	LYS	CA-C-N	7.90	127.57	119.19
48	BD	119	LYS	C-N-CA	7.90	127.57	119.19
81	Bp	21	CYS	CA-C-N	7.89	128.32	119.32
81	Bp	21	CYS	C-N-CA	7.89	128.32	119.32
10	AL	69	LYS	CA-C-N	7.77	127.67	120.21
10	AL	69	LYS	C-N-CA	7.77	127.67	120.21
37	B1	173	ASP	CA-C-N	7.71	127.36	119.19
37	B1	173	ASP	C-N-CA	7.71	127.36	119.19
16	AU	82	ASP	CA-C-N	7.63	127.17	118.85
16	AU	82	ASP	C-N-CA	7.63	127.17	118.85
87	Bx	135	LEU	CA-C-N	7.51	128.19	119.47
87	Bx	135	LEU	C-N-CA	7.51	128.19	119.47
56	BP	9	GLY	CA-C-N	7.49	129.20	119.84
56	BP	9	GLY	C-N-CA	7.49	129.20	119.84
57	BQ	211	ASN	CA-C-N	7.49	127.16	119.82
57	BQ	211	ASN	C-N-CA	7.49	127.16	119.82
66	Ba	338	GLN	CA-C-N	7.47	127.90	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
66	Ba	338	GLN	C-N-CA	7.47	127.90	119.83
54	BN	147	GLN	CA-C-N	7.47	127.14	119.82
54	BN	147	GLN	C-N-CA	7.47	127.14	119.82
52	BJ	158	GLU	CA-C-N	7.43	127.60	120.31
52	BJ	158	GLU	C-N-CA	7.43	127.60	120.31
49	BE	239	ARG	CA-C-N	7.38	127.05	119.82
49	BE	239	ARG	C-N-CA	7.38	127.05	119.82
22	Ad	44	THR	CA-C-N	7.37	125.04	119.66
22	Ad	44	THR	C-N-CA	7.37	125.04	119.66
30	Am	15	ASN	CA-C-N	7.28	126.91	119.19
30	Am	15	ASN	C-N-CA	7.28	126.91	119.19
8	AJ	68	GLU	CA-C-N	7.24	128.89	119.84
8	AJ	68	GLU	C-N-CA	7.24	128.89	119.84
79	Bn	76	GLY	CA-C-N	7.17	127.58	119.83
79	Bn	76	GLY	C-N-CA	7.17	127.58	119.83
36	B0	36	GLY	N-CA-C	7.16	121.06	111.03
33	Ap	229	GLY	CA-C-N	-7.10	113.07	120.38
33	Ap	229	GLY	C-N-CA	-7.10	113.07	120.38
40	B4	62	GLY	N-CA-C	-7.00	104.85	114.64
69	Bd	83	ILE	CA-C-N	6.87	127.11	119.90
69	Bd	83	ILE	C-N-CA	6.87	127.11	119.90
72	Bg	109	GLY	N-CA-C	-6.87	106.91	115.08
39	B3	41	ILE	CA-C-N	6.85	127.22	119.83
39	B3	41	ILE	C-N-CA	6.85	127.22	119.83
69	Bd	102	PRO	N-CA-C	6.79	118.99	110.70
56	BP	72	THR	CA-C-N	6.74	126.70	119.76
56	BP	72	THR	C-N-CA	6.74	126.70	119.76
41	B5	96	ASN	CA-C-N	6.69	126.64	119.28
41	B5	96	ASN	C-N-CA	6.69	126.64	119.28
60	BT	168	ASN	CA-C-N	6.68	126.31	119.56
60	BT	168	ASN	C-N-CA	6.68	126.31	119.56
40	B4	71	GLU	CA-C-N	6.68	126.36	119.82
40	B4	71	GLU	C-N-CA	6.68	126.36	119.82
54	BN	54	GLY	N-CA-C	-6.66	100.61	110.87
48	BD	123	PHE	N-CA-C	6.61	119.47	110.55
21	Ac	141	CYS	N-CA-C	-6.60	104.16	111.82
50	BF	121	ARG	N-CA-C	6.59	119.02	111.11
70	Be	129	TYR	CA-C-N	-6.58	113.02	119.87
70	Be	129	TYR	C-N-CA	-6.58	113.02	119.87
77	Bl	77	ASP	CA-C-N	-6.54	113.78	120.85
77	Bl	77	ASP	C-N-CA	-6.54	113.78	120.85
49	BE	252	TRP	CA-C-N	6.53	126.22	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	BE	252	TRP	C-N-CA	6.53	126.22	119.56
31	An	191	THR	CA-C-N	6.49	126.51	119.89
31	An	191	THR	C-N-CA	6.49	126.51	119.89
48	BD	183	HIS	N-CA-C	6.49	115.78	108.25
49	BE	339	GLN	CA-C-N	6.48	126.17	119.56
49	BE	339	GLN	C-N-CA	6.48	126.17	119.56
62	BV	72	ASP	CA-C-N	6.46	126.97	119.47
62	BV	72	ASP	C-N-CA	6.46	126.97	119.47
32	Ao	124	TYR	CA-C-N	6.45	125.88	118.85
32	Ao	124	TYR	C-N-CA	6.45	125.88	118.85
83	Bt	64	ALA	N-CA-C	-6.40	105.50	113.38
5	AF	105	CYS	N-CA-C	-6.40	100.43	109.96
75	Bj	208	ALA	CA-C-N	6.38	126.56	120.31
75	Bj	208	ALA	C-N-CA	6.38	126.56	120.31
44	B8	113	ARG	N-CA-C	6.35	121.17	113.17
87	Bx	164	ASN	N-CA-C	6.34	121.15	113.17
20	Ab	39	PRO	CA-C-N	6.30	126.26	120.21
20	Ab	39	PRO	C-N-CA	6.30	126.26	120.21
66	Ba	277	THR	N-CA-C	-6.29	100.19	109.81
3	AC	127	LEU	CA-C-N	6.28	124.18	119.66
3	AC	127	LEU	C-N-CA	6.28	124.18	119.66
60	BT	194	LEU	CA-C-N	6.28	126.47	119.32
60	BT	194	LEU	C-N-CA	6.28	126.47	119.32
84	Bu	49	TYR	CA-C-N	6.28	125.84	119.19
84	Bu	49	TYR	C-N-CA	6.28	125.84	119.19
39	B3	124	LEU	CA-C-N	6.26	126.00	119.05
39	B3	124	LEU	C-N-CA	6.26	126.00	119.05
7	AI	145	ARG	CA-C-N	6.23	125.99	119.76
7	AI	145	ARG	C-N-CA	6.23	125.99	119.76
36	B0	107	ASN	CA-C-N	6.22	125.91	119.56
36	B0	107	ASN	C-N-CA	6.22	125.91	119.56
71	Bf	67	ILE	CA-C-N	6.21	126.16	119.76
71	Bf	67	ILE	C-N-CA	6.21	126.16	119.76
39	B3	113	VAL	N-CA-C	6.21	118.13	112.29
10	AL	44	HIS	CA-C-N	6.20	126.77	120.38
10	AL	44	HIS	C-N-CA	6.20	126.77	120.38
15	AR	90	GLY	N-CA-C	-6.20	106.59	115.64
87	Bx	174	MET	CA-C-N	6.16	126.37	119.90
87	Bx	174	MET	C-N-CA	6.16	126.37	119.90
2	AB	183	GLY	CA-C-N	6.15	126.33	119.32
2	AB	183	GLY	C-N-CA	6.15	126.33	119.32
49	BE	316	PHE	N-CA-C	6.14	120.49	108.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	B0	95	GLY	N-CA-C	6.12	118.84	110.58
48	BD	133	ASP	CA-C-N	6.11	125.67	119.19
48	BD	133	ASP	C-N-CA	6.11	125.67	119.19
52	BJ	171	ILE	CA-C-N	6.08	125.70	119.56
52	BJ	171	ILE	C-N-CA	6.08	125.70	119.56
63	BW	182	PRO	CA-C-N	6.06	126.37	119.83
63	BW	182	PRO	C-N-CA	6.06	126.37	119.83
12	AO	69	PRO	CA-C-N	6.05	126.49	119.47
12	AO	69	PRO	C-N-CA	6.05	126.49	119.47
49	BE	230	THR	N-CA-C	6.05	120.94	113.50
56	BP	84	ASN	N-CA-C	-6.04	105.77	113.02
66	Ba	347	THR	N-CA-C	6.03	119.07	108.75
60	BT	262	GLN	CA-C-N	6.01	126.18	119.32
60	BT	262	GLN	C-N-CA	6.01	126.18	119.32
53	BK	84	GLN	CA-C-N	6.01	125.97	119.78
53	BK	84	GLN	C-N-CA	6.01	125.97	119.78
65	BY	25	ARG	CA-C-N	6.00	126.42	119.47
65	BY	25	ARG	C-N-CA	6.00	126.42	119.47
6	AG	193	GLU	N-CA-C	5.98	117.67	111.03
80	Bo	48	ASP	N-CA-C	5.98	120.05	112.87
33	Ap	167	ILE	CA-C-N	5.97	125.94	120.21
33	Ap	167	ILE	C-N-CA	5.97	125.94	120.21
55	BO	58	ILE	CB-CA-C	-5.93	106.67	111.71
68	Bc	131	ASP	CA-C-N	5.90	125.60	119.82
68	Bc	131	ASP	C-N-CA	5.90	125.60	119.82
33	Ap	207	GLN	CA-C-N	5.88	126.44	120.38
33	Ap	207	GLN	C-N-CA	5.88	126.44	120.38
76	Bk	147	ASP	N-CA-C	5.87	118.33	109.23
9	AK	188	CYS	N-CA-C	5.85	118.49	110.24
82	Bq	102	GLY	CA-C-N	5.83	126.39	120.38
82	Bq	102	GLY	C-N-CA	5.83	126.39	120.38
29	Ak	97	VAL	N-CA-C	5.80	113.80	107.60
57	BQ	69	LEU	N-CA-C	-5.79	105.71	112.89
5	AF	90	ARG	CA-C-N	5.79	126.28	120.14
5	AF	90	ARG	C-N-CA	5.79	126.28	120.14
9	AK	66	PRO	N-CA-C	5.79	117.76	110.70
9	AK	121	ASN	N-CA-C	5.79	118.33	111.33
50	BF	154	GLY	CA-C-N	5.77	125.97	120.31
50	BF	154	GLY	C-N-CA	5.77	125.97	120.31
2	AB	242	PRO	N-CA-C	5.76	117.72	110.70
86	Bw	88	PHE	N-CA-C	5.75	117.32	110.19
7	AI	374	ASP	CA-C-N	5.75	125.45	119.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	AI	374	ASP	C-N-CA	5.75	125.45	119.82
49	BE	78	CYS	CA-C-N	5.74	125.10	118.85
49	BE	78	CYS	C-N-CA	5.74	125.10	118.85
56	BP	143	GLU	N-CA-C	5.74	117.99	111.11
52	BJ	139	LYS	N-CA-C	5.73	118.74	111.69
13	AP	100	HIS	CA-C-N	5.71	125.56	119.28
13	AP	100	HIS	C-N-CA	5.71	125.56	119.28
5	AF	96	HIS	CA-C-N	5.71	126.09	119.47
5	AF	96	HIS	C-N-CA	5.71	126.09	119.47
70	Be	26	GLY	CA-C-N	5.70	126.97	119.84
70	Be	26	GLY	C-N-CA	5.70	126.97	119.84
67	Bb	93	PRO	CA-C-N	5.69	126.24	120.38
67	Bb	93	PRO	C-N-CA	5.69	126.24	120.38
68	Bc	263	GLY	CA-C-N	5.67	125.87	120.31
68	Bc	263	GLY	C-N-CA	5.67	125.87	120.31
74	Bi	195	VAL	N-CA-C	5.67	116.32	110.82
15	AR	57	ASN	CA-C-N	5.65	125.18	119.19
15	AR	57	ASN	C-N-CA	5.65	125.18	119.19
41	B5	107	ILE	N-CA-C	5.65	116.36	109.30
79	Bn	118	TYR	N-CA-C	-5.65	104.81	110.97
39	B3	117	ILE	N-CA-C	5.65	116.84	108.65
44	B8	180	TYR	N-CA-C	5.64	120.16	113.28
50	BF	129	VAL	CB-CA-C	-5.62	105.15	111.45
75	Bj	170	ILE	N-CA-C	5.62	115.95	107.75
86	Bw	279	GLY	N-CA-C	-5.62	108.01	114.69
72	Bg	123	SER	CA-C-N	5.61	125.70	119.87
72	Bg	123	SER	C-N-CA	5.61	125.70	119.87
26	Ah	324	ILE	N-CA-C	5.60	115.79	110.42
72	Bg	82	GLY	N-CA-C	-5.59	107.94	115.21
4	AE	378	GLY	CA-C-N	5.56	125.65	119.87
4	AE	378	GLY	C-N-CA	5.56	125.65	119.87
67	Bb	351	HIS	CA-C-N	5.55	125.86	119.92
67	Bb	351	HIS	C-N-CA	5.55	125.86	119.92
67	Bb	256	PRO	CA-C-N	5.54	125.86	119.93
67	Bb	256	PRO	C-N-CA	5.54	125.86	119.93
46	BA	68	A	P-O3'-C3'	5.54	128.51	120.20
13	AP	55	ASP	CA-C-N	5.54	124.73	118.97
13	AP	55	ASP	C-N-CA	5.54	124.73	118.97
37	B1	141	PHE	N-CA-C	-5.50	105.20	111.14
39	B3	39	SER	CB-CA-C	-5.48	109.27	115.79
49	BE	345	ILE	N-CA-C	5.47	117.34	109.51
52	BJ	71	PRO	N-CA-C	5.46	117.36	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BN	171	SER	CA-C-N	5.46	123.65	119.66
54	BN	171	SER	C-N-CA	5.46	123.65	119.66
73	Bh	286	GLY	N-CA-C	5.46	118.69	110.18
39	B3	37	THR	N-CA-C	5.45	115.32	108.45
46	BA	330	A	N9-C1'-C2'	-5.45	105.82	114.00
68	Bc	130	ASP	N-CA-C	5.45	117.22	111.28
49	BE	244	SER	N-CA-C	5.44	115.42	108.24
74	Bi	191	PRO	CA-C-N	5.43	125.74	119.93
74	Bi	191	PRO	C-N-CA	5.43	125.74	119.93
75	Bj	61	LYS	CA-C-N	5.43	125.43	120.21
75	Bj	61	LYS	C-N-CA	5.43	125.43	120.21
66	Ba	360	ASN	N-CA-C	5.42	120.05	113.38
6	AG	53	LYS	CA-C-N	5.42	124.94	119.19
6	AG	53	LYS	C-N-CA	5.42	124.94	119.19
21	Ac	125	HIS	CA-C-N	5.42	124.93	119.19
21	Ac	125	HIS	C-N-CA	5.42	124.93	119.19
58	BR	129	ASN	CA-C-N	-5.39	115.36	122.85
58	BR	129	ASN	C-N-CA	-5.39	115.36	122.85
69	Bd	175	GLY	CA-C-N	5.39	125.69	119.92
69	Bd	175	GLY	C-N-CA	5.39	125.69	119.92
72	Bg	72	VAL	CA-C-N	5.39	125.70	119.93
72	Bg	72	VAL	C-N-CA	5.39	125.70	119.93
28	Aj	116	GLY	N-CA-C	5.39	120.25	112.81
48	BD	121	GLY	CA-C-N	5.38	125.65	119.83
48	BD	121	GLY	C-N-CA	5.38	125.65	119.83
44	B8	131	LYS	N-CA-C	5.38	117.29	108.52
43	B7	55	GLU	N-CA-C	5.38	118.63	111.75
15	AR	86	SER	CA-C-N	5.37	124.55	118.97
15	AR	86	SER	C-N-CA	5.37	124.55	118.97
54	BN	166	PHE	CA-C-N	5.36	125.12	119.76
54	BN	166	PHE	C-N-CA	5.36	125.12	119.76
2	AB	227	ASN	CA-C-N	5.35	124.86	119.19
2	AB	227	ASN	C-N-CA	5.35	124.86	119.19
68	Bc	106	ASP	CB-CA-C	-5.34	109.96	117.23
68	Bc	122	ILE	N-CA-C	5.34	115.65	108.17
24	Af	88	SER	CA-C-N	5.34	126.52	119.84
24	Af	88	SER	C-N-CA	5.34	126.52	119.84
66	Ba	330	GLY	N-CA-C	5.34	117.49	112.04
64	BX	63	VAL	CA-C-N	5.33	126.50	119.84
64	BX	63	VAL	C-N-CA	5.33	126.50	119.84
49	BE	323	GLY	N-CA-C	5.32	119.12	112.73
54	BN	112	LEU	CA-C-N	-5.32	114.76	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BN	112	LEU	C-N-CA	-5.32	114.76	120.03
67	Bb	67	LYS	CA-C-N	5.32	126.49	119.84
67	Bb	67	LYS	C-N-CA	5.32	126.49	119.84
32	Ao	92	ASP	CA-C-N	5.32	125.64	119.47
32	Ao	92	ASP	C-N-CA	5.32	125.64	119.47
21	Ac	5	GLY	N-CA-C	-5.32	105.05	112.18
56	BP	54	LYS	CB-CA-C	-5.29	108.93	116.34
74	Bi	89	VAL	CA-C-N	5.29	125.83	120.38
74	Bi	89	VAL	C-N-CA	5.29	125.83	120.38
46	BA	512	A	P-O3'-C3'	5.28	128.11	120.20
68	Bc	244	ASN	CA-C-N	5.27	125.59	119.47
68	Bc	244	ASN	C-N-CA	5.27	125.59	119.47
53	BK	36	GLY	CA-C-N	5.27	124.60	118.85
53	BK	36	GLY	C-N-CA	5.27	124.60	118.85
49	BE	201	GLY	N-CA-C	-5.27	100.69	113.18
85	Bv	66	ALA	N-CA-C	-5.25	105.20	111.03
3	AC	58	ALA	CA-C-N	5.22	125.53	119.47
3	AC	58	ALA	C-N-CA	5.22	125.53	119.47
81	Bp	70	ASP	N-CA-C	-5.21	106.90	113.20
86	Bw	100	LEU	CA-C-N	-5.21	115.27	123.13
86	Bw	100	LEU	C-N-CA	-5.21	115.27	123.13
49	BE	282	ILE	N-CA-C	5.20	115.47	107.77
33	Ap	235	MET	N-CA-C	5.20	119.31	112.35
69	Bd	90	THR	CA-C-N	5.20	125.13	119.78
69	Bd	90	THR	C-N-CA	5.20	125.13	119.78
14	AQ	79	HIS	N-CA-C	5.18	117.28	109.41
67	Bb	185	MET	CA-C-N	5.18	125.39	120.31
67	Bb	185	MET	C-N-CA	5.18	125.39	120.31
86	Bw	357	ASP	N-CA-C	-5.18	101.26	109.96
87	Bx	63	PRO	CA-C-N	5.18	124.80	119.05
87	Bx	63	PRO	C-N-CA	5.18	124.80	119.05
10	AL	72	LYS	N-CA-C	5.17	119.53	112.55
75	Bj	146	ARG	N-CA-C	-5.17	106.83	113.23
28	Aj	55	TRP	N-CA-C	5.16	116.59	110.97
48	BD	291	PRO	O-C-N	5.16	123.57	121.15
65	BY	129	LYS	CA-C-N	5.15	124.91	119.76
65	BY	129	LYS	C-N-CA	5.15	124.91	119.76
66	Ba	52	ILE	N-CA-C	5.15	113.11	107.60
13	AP	37	ALA	N-CA-C	5.14	114.93	108.45
79	Bn	46	ARG	N-CA-C	-5.13	106.79	113.16
6	AG	136	THR	N-CA-C	5.13	116.68	111.14
59	BS	66	ARG	N-CA-C	-5.13	102.89	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	B5	80	ALA	CA-C-N	5.11	125.40	119.93
41	B5	80	ALA	C-N-CA	5.11	125.40	119.93
46	BA	931	A	P-O3'-C3'	5.11	127.87	120.20
12	AO	67	ASP	CA-C-N	5.11	125.64	120.38
12	AO	67	ASP	C-N-CA	5.11	125.64	120.38
54	BN	128	PHE	CA-C-N	5.11	125.14	119.32
54	BN	128	PHE	C-N-CA	5.11	125.14	119.32
64	BX	100	ALA	N-CA-C	5.11	117.63	111.40
28	Aj	112	GLY	N-CA-C	5.09	117.91	110.38
49	BE	337	VAL	N-CA-C	5.08	115.63	108.36
28	Aj	188	GLU	CA-C-N	5.08	126.19	119.84
28	Aj	188	GLU	C-N-CA	5.08	126.19	119.84
36	B0	38	SER	N-CA-C	5.07	117.69	110.24
48	BD	93	VAL	N-CA-C	5.06	115.33	107.28
26	Ah	337	GLY	CA-C-N	5.06	124.67	119.56
26	Ah	337	GLY	C-N-CA	5.06	124.67	119.56
56	BP	69	GLY	N-CA-C	-5.06	106.16	114.76
60	BT	235	ARG	CA-C-N	5.06	124.72	119.56
60	BT	235	ARG	C-N-CA	5.06	124.72	119.56
70	Be	46	GLY	N-CA-C	-5.06	107.56	114.64
43	B7	68	GLY	N-CA-C	5.05	117.27	111.36
3	AC	166	TYR	CB-CA-C	-5.05	109.27	116.34
49	BE	341	GLY	N-CA-C	-5.03	101.27	113.18
50	BF	125	ARG	N-CA-C	5.01	116.86	108.99
86	Bw	186	ASN	CA-C-N	5.01	124.67	119.56
86	Bw	186	ASN	C-N-CA	5.01	124.67	119.56

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	AK	194	ARG	Peptide
49	BE	316	PHE	Peptide
57	BQ	149	HIS	Peptide
60	BT	275	THR	Peptide
67	Bb	164	GLY	Peptide
67	Bb	210	GLU	Peptide
79	Bn	65	ASN	Peptide
83	Bt	62	HIS	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	20411	0	10345	375	0
2	AB	1762	0	1774	63	0
3	AC	1075	0	1087	48	0
4	AE	2621	0	2640	111	0
5	AF	990	0	1025	41	0
6	AG	1721	0	1747	53	0
7	AI	2498	0	2473	88	0
8	AJ	1067	0	1101	55	0
9	AK	1001	0	1037	42	0
10	AL	840	0	890	27	0
11	AN	858	0	883	46	0
12	AO	1448	0	1536	38	0
13	AP	932	0	951	43	0
14	AQ	853	0	913	46	0
15	AR	784	0	813	35	0
16	AU	734	0	745	32	0
17	AV	1251	0	823	72	0
17	AY	1251	0	824	77	0
18	AX	231	0	157	7	0
19	Aa	2296	0	2317	166	0
20	Ab	1101	0	1118	33	0
21	Ac	1367	0	1385	56	0
22	Ad	1467	0	1466	49	0
23	Ae	2016	0	2028	447	0
24	Af	778	0	791	34	0
25	Ag	2774	0	2810	146	0
26	Ah	876	0	832	32	0
27	Ai	824	0	842	32	0
28	Aj	1777	0	1788	72	0
29	Ak	2222	0	2270	88	0
30	Am	930	0	959	32	0
31	An	639	0	709	26	0
32	Ao	3028	0	3081	437	0
33	Ap	1551	0	1519	72	0
34	As	96	0	98	11	0
35	Az	102	0	104	25	0
36	B0	878	0	896	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	B1	2036	0	2058	66	0
38	B2	1544	0	1580	64	0
39	B3	968	0	1018	40	0
40	B4	381	0	400	19	0
41	B5	902	0	916	38	0
42	B6	391	0	429	27	0
43	B7	387	0	413	15	0
44	B8	833	0	883	45	0
45	B9	335	0	359	17	0
46	BA	32233	0	16311	725	0
47	BB	1008	0	555	32	0
48	BD	1860	0	1923	73	0
49	BE	2420	0	2418	114	0
50	BF	2011	0	2049	103	0
51	BI	805	0	845	25	0
52	BJ	1361	0	1448	52	0
53	BK	1081	0	1146	38	0
54	BN	1444	0	1437	73	0
55	BO	896	0	946	39	0
56	BP	2312	0	2373	130	0
57	BQ	1792	0	1832	54	0
58	BR	1240	0	1260	52	0
59	BS	1168	0	1159	74	0
60	BT	1950	0	1969	72	0
61	BU	1159	0	1228	58	0
62	BV	1231	0	1278	55	0
63	BW	1374	0	1405	56	0
64	BX	1120	0	1133	68	0
65	BY	1663	0	1665	67	0
66	Ba	3173	0	3153	121	0
67	Bb	2952	0	2840	134	0
68	Bc	2408	0	2415	95	0
69	Bd	832	0	828	50	0
70	Be	968	0	968	44	0
71	Bf	852	0	834	69	0
72	Bg	1167	0	1173	63	0
73	Bh	2319	0	2332	93	0
74	Bi	1979	0	1974	83	0
75	Bj	1775	0	1797	78	0
76	Bk	1087	0	1080	47	0
77	Bl	1097	0	1080	32	0
78	Bm	893	0	878	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
79	Bn	837	0	860	42	0
80	Bo	747	0	748	23	0
81	Bp	742	0	749	18	0
82	Bq	336	0	342	21	0
83	Bt	780	0	792	47	0
84	Bu	1208	0	1227	40	0
85	Bv	1068	0	1032	29	0
86	Bw	3126	0	3153	132	0
87	Bx	1325	0	1354	75	0
88	Bz	564	0	574	131	0
89	AA	146	0	0	0	0
89	Ag	1	0	0	0	0
89	B0	1	0	0	0	0
89	B2	1	0	0	0	0
89	BA	195	0	0	0	0
89	BD	2	0	0	0	0
89	BE	1	0	0	0	0
89	BP	1	0	0	0	0
89	BR	2	0	0	0	0
89	BX	1	0	0	0	0
90	AR	1	0	0	0	0
90	Ac	1	0	0	0	0
90	Ap	1	0	0	0	0
90	B5	1	0	0	0	0
90	B9	1	0	0	0	0
90	Bx	1	0	0	0	0
91	Ag	28	0	12	0	0
92	AA	114	0	0	7	0
92	Ag	4	0	0	1	0
92	B0	3	0	0	0	0
92	B7	2	0	0	0	0
92	B8	1	0	0	0	0
92	BA	196	0	0	12	0
92	BD	3	0	0	0	0
92	BF	4	0	0	0	0
92	BI	1	0	0	0	0
92	BO	2	0	0	0	0
92	BP	3	0	0	2	0
92	BR	2	0	0	0	0
92	BU	1	0	0	0	0
92	BW	4	0	0	0	0
All	All	167915	0	141408	5789	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (5789) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:Ao:558:UNK:HG1	32:Ao:576:UNK:CG	1.37	1.49
71:Bf:88:UNK:HG2	71:Bf:91:UNK:CG	1.44	1.43
32:Ao:558:UNK:CG	32:Ao:576:UNK:HG1	1.57	1.34
23:Ae:200:UNK:O	23:Ae:204:UNK:HG3	1.28	1.32
19:Aa:324:UNK:O	19:Aa:328:UNK:HG3	1.32	1.30
19:Aa:326:UNK:O	19:Aa:330:UNK:HG3	1.29	1.29
23:Ae:273:UNK:CG	23:Ae:276:UNK:HG3	1.65	1.25
23:Ae:70:UNK:O	23:Ae:73:UNK:HG3	1.34	1.25
71:Bf:92:UNK:O	71:Bf:95:UNK:HG3	1.33	1.22
71:Bf:88:UNK:CG	71:Bf:91:UNK:HG1	1.69	1.22
19:Aa:312:UNK:O	19:Aa:316:UNK:HG3	1.38	1.21
17:AV:54:Y5P:N3	17:AV:58:Y5P:H5	1.56	1.20
32:Ao:514:UNK:HG1	32:Ao:541:UNK:CG	1.72	1.19
92:AA:8117:HOH:O	17:AV:29:Y5P:H4A	1.44	1.17
32:Ao:373:UNK:HG3	34:As:2363:UNK:CG	1.74	1.17
23:Ae:63:UNK:CG	23:Ae:65:UNK:HG3	1.74	1.16
23:Ae:58:UNK:O	23:Ae:62:UNK:HG3	1.39	1.16
23:Ae:46:UNK:CG	23:Ae:77:UNK:CG	2.22	1.15
23:Ae:46:UNK:HG1	23:Ae:77:UNK:CG	1.75	1.15
23:Ae:391:UNK:O	23:Ae:394:UNK:HG3	1.44	1.15
25:Ag:63:UNK:O	25:Ag:64:UNK:HG3	1.46	1.15
88:Bz:31:UNK:O	88:Bz:34:UNK:HG3	1.38	1.15
25:Ag:52:UNK:HG2	25:Ag:66:UNK:HG3	1.25	1.15
32:Ao:373:UNK:CG	34:As:2363:UNK:HG1	1.76	1.15
23:Ae:181:UNK:CG	23:Ae:210:UNK:CG	2.24	1.13
32:Ao:476:UNK:HG1	32:Ao:510:UNK:N	1.63	1.13
19:Aa:329:UNK:O	19:Aa:333:UNK:HG3	1.48	1.12
32:Ao:476:UNK:HG1	32:Ao:510:UNK:H2	1.14	1.12
23:Ae:104:UNK:HG2	23:Ae:107:UNK:HG3	1.23	1.12
23:Ae:167:UNK:CG	23:Ae:205:UNK:HG2	1.79	1.12
23:Ae:233:UNK:O	23:Ae:236:UNK:HG3	1.50	1.12
67:Bb:155:CYS:O	67:Bb:267:ARG:NH1	1.83	1.11
32:Ao:359:UNK:HG2	32:Ao:396:UNK:HG1	1.31	1.11
23:Ae:174:UNK:CG	23:Ae:176:UNK:HG3	1.79	1.10
23:Ae:181:UNK:HG1	23:Ae:210:UNK:CG	1.80	1.10
27:Ai:17:ARG:NH2	35:Az:698:UNK:HG3	1.66	1.10
19:Aa:331:UNK:HG2	19:Aa:341:UNK:HG2	1.25	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Ae:230:UNK:O	23:Ae:231:UNK:HG3	1.52	1.09
32:Ao:338:UNK:CG	32:Ao:365:UNK:HG1	1.83	1.09
88:Bz:22:UNK:O	88:Bz:26:UNK:HG3	1.52	1.08
23:Ae:174:UNK:CG	23:Ae:176:UNK:CG	2.31	1.08
23:Ae:197:UNK:CG	23:Ae:230:UNK:HG1	1.82	1.08
23:Ae:167:UNK:HG1	23:Ae:205:UNK:CG	1.84	1.08
19:Aa:314:UNK:O	19:Aa:318:UNK:HG3	1.54	1.07
35:Az:703:UNK:O	35:Az:707:UNK:HG2	1.51	1.07
23:Ae:219:UNK:O	23:Ae:223:UNK:HG3	1.54	1.07
23:Ae:400:UNK:O	23:Ae:403:UNK:HG3	1.53	1.07
32:Ao:581:UNK:HG1	32:Ao:654:UNK:HG2	1.29	1.07
70:Be:44:ARG:HH12	86:Bw:157:ALA:HB3	1.19	1.07
32:Ao:339:UNK:HG2	32:Ao:376:UNK:HB1	1.32	1.06
19:Aa:331:UNK:HG2	19:Aa:341:UNK:CG	1.85	1.06
32:Ao:161:UNK:O	32:Ao:165:UNK:HG3	1.56	1.06
23:Ae:208:UNK:HG2	23:Ae:220:UNK:HG1	1.29	1.05
44:B8:142:ARG:NH1	46:BA:1191:C:OP2	1.90	1.05
23:Ae:170:UNK:HG2	23:Ae:170:UNK:O	1.54	1.05
23:Ae:273:UNK:CG	23:Ae:276:UNK:CG	2.34	1.05
23:Ae:105:UNK:O	23:Ae:109:UNK:HG3	1.56	1.05
32:Ao:514:UNK:CG	32:Ao:541:UNK:HG1	1.85	1.05
53:BK:124:LYS:NZ	53:BK:127:ASP:OD2	1.89	1.05
32:Ao:462:UNK:O	32:Ao:466:UNK:HG3	1.56	1.05
23:Ae:243:UNK:HG2	23:Ae:245:UNK:HG3	1.35	1.04
23:Ae:268:UNK:HG3	33:Ap:214:SER:OG	1.56	1.04
88:Bz:24:UNK:O	88:Bz:27:UNK:HG3	1.56	1.04
32:Ao:196:UNK:CG	32:Ao:206:UNK:HG1	1.88	1.04
66:Ba:153:ARG:HH22	86:Bw:191:ALA:HA	1.21	1.04
32:Ao:194:UNK:HA	32:Ao:230:UNK:HG1	1.38	1.03
32:Ao:521:UNK:HG1	32:Ao:534:UNK:CG	1.88	1.03
73:Bh:259:ARG:HG3	73:Bh:259:ARG:HH11	1.16	1.03
32:Ao:373:UNK:CG	34:As:2363:UNK:CG	2.35	1.03
23:Ae:273:UNK:HG2	23:Ae:276:UNK:HG3	1.03	1.02
32:Ao:581:UNK:HG1	32:Ao:654:UNK:CG	1.87	1.02
23:Ae:222:UNK:O	23:Ae:225:UNK:HG3	1.58	1.02
19:Aa:343:UNK:O	19:Aa:346:UNK:HG3	1.58	1.02
55:BO:72:ARG:HB2	55:BO:72:ARG:HH11	1.22	1.02
23:Ae:188:UNK:O	23:Ae:192:UNK:HG3	1.60	1.02
88:Bz:13:UNK:O	88:Bz:16:UNK:HG3	1.59	1.02
32:Ao:558:UNK:HG1	32:Ao:576:UNK:HG3	1.42	1.01
23:Ae:181:UNK:HG2	23:Ae:210:UNK:HG1	1.42	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Ac:36:THR:H	21:Ac:69:ASN:HD21	1.08	1.01
32:Ao:304:UNK:O	32:Ao:307:UNK:HG3	1.61	1.01
1:AA:209:C:H4'	13:AP:43:ARG:HH12	1.19	1.01
23:Ae:134:UNK:O	23:Ae:135:UNK:HG3	1.57	1.01
32:Ao:476:UNK:HB2	32:Ao:513:UNK:HG1	1.38	1.01
67:Bb:308:GLN:O	80:Bo:113:LYS:NZ	1.94	1.01
19:Aa:307:HIS:O	19:Aa:313:UNK:HG1	1.60	1.01
23:Ae:174:UNK:HG2	23:Ae:176:UNK:HG3	1.41	1.00
88:Bz:17:UNK:O	88:Bz:21:UNK:HG3	1.61	1.00
38:B2:93:ARG:NH1	70:Be:82:THR:O	1.93	1.00
88:Bz:409:UNK:O	88:Bz:412:UNK:HG3	1.61	1.00
19:Aa:350:UNK:O	19:Aa:353:UNK:HG3	1.60	1.00
23:Ae:273:UNK:O	23:Ae:277:UNK:HG3	1.62	1.00
17:AY:6:Y5P:H4A	17:AY:7:Y5P:H4	1.40	0.99
17:AV:55:Y5P:C2'	17:AV:57:Y5P:H5	1.93	0.99
32:Ao:485:UNK:O	32:Ao:489:UNK:HG3	1.62	0.99
8:AJ:64:THR:HG22	32:Ao:64:THR:O	1.63	0.99
48:BD:263:ARG:HH11	48:BD:263:ARG:HB2	1.24	0.99
32:Ao:338:UNK:HG1	32:Ao:365:UNK:HG1	1.39	0.99
17:AY:70:Y5P:H4A	17:AY:71:Y5P:H4	1.45	0.99
47:BB:65:Y5P:H2'	47:BB:66:P5P:H8	1.45	0.99
23:Ae:243:UNK:CG	23:Ae:245:UNK:HG3	1.93	0.98
32:Ao:420:UNK:HB2	32:Ao:459:UNK:HG1	1.43	0.98
17:AY:25:Y5P:H4A	17:AY:26:Y5P:H4	1.43	0.98
23:Ae:197:UNK:HG1	23:Ae:230:UNK:HG1	1.41	0.98
27:Ai:13:ARG:HH22	35:Az:692:UNK:HG2	1.23	0.98
23:Ae:174:UNK:HG1	23:Ae:176:UNK:CG	1.93	0.98
32:Ao:396:UNK:O	32:Ao:399:UNK:HG3	1.64	0.98
32:Ao:539:UNK:HG3	32:Ao:583:UNK:HG1	1.45	0.97
32:Ao:427:UNK:HG1	32:Ao:463:UNK:HA	1.47	0.97
32:Ao:538:UNK:O	32:Ao:550:UNK:HG1	1.63	0.96
32:Ao:458:UNK:O	32:Ao:461:UNK:HG3	1.64	0.96
19:Aa:338:UNK:O	19:Aa:342:UNK:HG3	1.64	0.96
32:Ao:521:UNK:HG1	32:Ao:534:UNK:HG2	1.47	0.96
46:BA:62:C:OP1	51:BI:76:ARG:NH1	1.99	0.96
61:BU:54:THR:HG21	62:BV:176:MET:H	1.27	0.96
1:AA:393:A:OP1	12:AO:136:LYS:NZ	1.99	0.96
46:BA:79:U:O2'	51:BI:61:LYS:NZ	1.98	0.96
19:Aa:310:UNK:CG	19:Aa:313:UNK:HG2	1.96	0.96
44:B8:132:LYS:HE3	46:BA:1230:G:H5'	1.48	0.95
23:Ae:46:UNK:CG	23:Ae:77:UNK:HG2	1.94	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Ae:139:UNK:HG3	23:Ae:140:UNK:N	1.81	0.95
23:Ae:306:UNK:O	23:Ae:309:UNK:HG3	1.65	0.95
7:AI:255:UNK:HG1	7:AI:371:LEU:HD13	1.48	0.95
23:Ae:181:UNK:CG	23:Ae:210:UNK:HG1	1.94	0.95
32:Ao:197:UNK:HG1	32:Ao:230:UNK:HG2	1.48	0.95
32:Ao:537:UNK:O	32:Ao:541:UNK:HG3	1.66	0.95
46:BA:346:U:H4'	46:BA:347:G:H5'	1.49	0.95
23:Ae:267:UNK:HG2	23:Ae:270:UNK:HG3	1.46	0.95
50:BF:257:GLN:O	56:BP:21:ARG:NH1	2.00	0.95
23:Ae:63:UNK:HG3	23:Ae:65:UNK:HG3	1.46	0.94
23:Ae:46:UNK:HG3	23:Ae:77:UNK:CG	1.94	0.94
32:Ao:360:UNK:O	32:Ao:363:UNK:HG3	1.67	0.94
1:AA:59:C:H42	28:Aj:133:GLN:HG2	1.31	0.94
32:Ao:514:UNK:HG1	32:Ao:541:UNK:HG1	0.95	0.94
54:BN:140:ASN:HB3	73:Bh:262:GLY:HA2	1.49	0.94
88:Bz:414:UNK:O	88:Bz:418:UNK:HG3	1.67	0.94
17:AV:37:Y5P:H4A	17:AV:38:Y5P:H4	1.48	0.94
88:Bz:605:UNK:O	88:Bz:608:UNK:HG3	1.68	0.94
17:AY:54:Y5P:N3	17:AY:58:Y5P:C5	2.31	0.94
23:Ae:273:UNK:HG3	23:Ae:276:UNK:CG	1.98	0.94
23:Ae:81:UNK:O	23:Ae:82:UNK:HG3	1.66	0.93
46:BA:463:U:OP1	83:Bt:23:ARG:NH2	2.01	0.93
49:BE:341:GLY:HA2	60:BT:105:ILE:HD11	1.49	0.93
6:AG:197:ARG:HB3	6:AG:197:ARG:HH11	1.33	0.93
73:Bh:105:ARG:HH11	73:Bh:116:LEU:HD23	1.33	0.93
69:Bd:167:SER:O	75:Bj:203:LYS:NZ	2.00	0.93
71:Bf:88:UNK:CG	71:Bf:91:UNK:CG	2.36	0.93
21:Ac:36:THR:O	21:Ac:45:ARG:NH1	2.00	0.93
23:Ae:354:UNK:HG2	23:Ae:357:UNK:HG3	1.49	0.93
32:Ao:656:UNK:O	32:Ao:660:UNK:HG3	1.69	0.93
23:Ae:46:UNK:CG	23:Ae:77:UNK:HG1	1.96	0.93
32:Ao:535:UNK:HG2	32:Ao:554:UNK:HG2	1.51	0.93
32:Ao:359:UNK:CG	32:Ao:396:UNK:HG1	1.97	0.93
19:Aa:311:UNK:HG2	19:Aa:312:UNK:N	1.83	0.93
16:AU:52:ARG:HH11	16:AU:52:ARG:HB2	1.34	0.92
28:Aj:27:ARG:HH12	28:Aj:33:ARG:NH1	1.67	0.92
23:Ae:181:UNK:HG1	23:Ae:210:UNK:HG2	1.50	0.92
32:Ao:558:UNK:CG	32:Ao:576:UNK:CG	2.31	0.92
3:AC:93:ARG:NH1	3:AC:108:LEU:O	2.03	0.92
23:Ae:354:UNK:CG	23:Ae:357:UNK:HG3	2.00	0.92
32:Ao:539:UNK:CG	32:Ao:583:UNK:HG1	1.99	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:Bb:47:ARG:HE	76:Bk:120:LYS:HZ1	0.97	0.92
27:Ai:13:ARG:HH22	35:Az:692:UNK:CG	1.83	0.92
34:As:2361:UNK:O	34:As:2364:UNK:HG3	1.71	0.92
50:BF:59:ARG:HG2	50:BF:59:ARG:HH11	1.36	0.91
71:Bf:88:UNK:HG2	71:Bf:91:UNK:HG3	1.51	0.91
75:Bj:185:ARG:NH1	75:Bj:206:GLY:O	2.03	0.91
23:Ae:61:UNK:HG1	23:Ae:94:UNK:CG	2.00	0.91
32:Ao:157:UNK:HG2	32:Ao:173:UNK:HG2	1.51	0.91
76:Bk:135:LEU:HD12	88:Bz:105:UNK:HG3	1.51	0.91
7:AI:253:UNK:HG3	7:AI:366:ARG:HH12	1.35	0.91
17:AY:54:Y5P:N3	17:AY:58:Y5P:H5	1.86	0.91
46:BA:618:A:HO2'	46:BA:619:U:H6	0.95	0.91
56:BP:137:GLY:HA3	56:BP:157:GLN:HG3	1.52	0.91
32:Ao:357:UNK:O	32:Ao:361:UNK:HG3	1.70	0.90
33:Ap:60:ASP:OD1	33:Ap:121:LYS:NZ	2.03	0.90
59:BS:178:ILE:HD11	84:Bu:176:ARG:HH12	1.37	0.90
32:Ao:175:UNK:O	32:Ao:178:UNK:HG3	1.70	0.90
60:BT:66:UNK:HG3	60:BT:66:UNK:O	1.72	0.89
21:Ac:132:ARG:NH1	21:Ac:136:LEU:O	2.05	0.89
66:Ba:333:SER:HB3	66:Ba:363:ASP:HB3	1.52	0.89
88:Bz:405:UNK:O	88:Bz:408:UNK:HG3	1.72	0.89
41:B5:152:PRO:HG3	41:B5:173:ARG:NH1	1.88	0.89
32:Ao:392:UNK:O	32:Ao:395:UNK:HG3	1.71	0.89
46:BA:1230:G:O2'	46:BA:1246:C:N4	2.05	0.89
32:Ao:374:UNK:O	32:Ao:378:UNK:HG3	1.71	0.89
23:Ae:69:UNK:HG1	23:Ae:103:UNK:HA	1.54	0.89
23:Ae:125:UNK:O	23:Ae:128:UNK:HG3	1.71	0.89
88:Bz:106:UNK:HG3	88:Bz:106:UNK:O	1.71	0.89
71:Bf:88:UNK:O	71:Bf:91:UNK:HG3	1.71	0.88
19:Aa:331:UNK:CG	19:Aa:341:UNK:HG2	2.03	0.88
20:Ab:68:ASP:OD1	20:Ab:71:ARG:NH1	2.05	0.88
32:Ao:225:UNK:HB1	32:Ao:248:UNK:HG1	1.51	0.88
23:Ae:218:UNK:HB1	23:Ae:256:UNK:HG1	1.55	0.88
32:Ao:414:UNK:O	32:Ao:417:UNK:HG3	1.74	0.88
23:Ae:61:UNK:HG1	23:Ae:94:UNK:HG2	1.56	0.88
23:Ae:233:UNK:O	23:Ae:236:UNK:CG	2.21	0.88
23:Ae:391:UNK:O	23:Ae:394:UNK:CG	2.22	0.88
48:BD:111:ARG:NH1	48:BD:182:ALA:HB2	1.88	0.88
32:Ao:190:UNK:HG1	32:Ao:223:UNK:O	1.71	0.88
71:Bf:87:UNK:HG2	71:Bf:88:UNK:HG3	1.52	0.88
23:Ae:70:UNK:O	23:Ae:73:UNK:CG	2.21	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:Ao:519:UNK:O	32:Ao:523:UNK:HG3	1.73	0.87
46:BA:100:C:O2'	79:Bn:75:LYS:NZ	2.06	0.87
67:Bb:234:HIS:O	67:Bb:296:ARG:NH1	2.08	0.87
70:Be:21:TRP:O	70:Be:32:LYS:NZ	2.07	0.87
1:AA:882:A:OP1	23:Ae:68:UNK:CG	2.22	0.87
19:Aa:311:UNK:O	19:Aa:315:UNK:HG3	1.75	0.87
56:BP:11:ARG:HG2	56:BP:11:ARG:HH11	1.38	0.87
38:B2:182:LYS:NZ	46:BA:28:A:OP2	2.06	0.87
17:AV:10:Y5P:O2'	88:Bz:425:UNK:HG1	1.73	0.87
32:Ao:232:UNK:HB2	32:Ao:241:UNK:HG1	1.55	0.87
32:Ao:535:UNK:CG	32:Ao:554:UNK:HG2	2.04	0.87
32:Ao:514:UNK:HB2	32:Ao:537:UNK:HG3	1.57	0.87
54:BN:74:GLN:HE22	87:Bx:175:PRO:HD2	1.39	0.87
2:AB:238:ASN:OD1	24:Af:120:LYS:NZ	2.08	0.86
48:BD:111:ARG:HH11	48:BD:182:ALA:HB2	1.37	0.86
32:Ao:373:UNK:HG3	34:As:2363:UNK:HG1	0.91	0.86
88:Bz:417:UNK:O	88:Bz:420:UNK:HG3	1.75	0.86
1:AA:273:A:OP1	33:Ap:92:LYS:NZ	2.08	0.86
17:AV:54:Y5P:N3	17:AV:58:Y5P:C5	2.39	0.86
59:BS:86:THR:HG22	59:BS:88:HIS:H	1.38	0.86
67:Bb:47:ARG:HE	76:Bk:120:LYS:NZ	1.74	0.86
23:Ae:175:UNK:O	23:Ae:179:UNK:HG2	1.75	0.86
23:Ae:197:UNK:HG2	23:Ae:230:UNK:HG1	1.58	0.86
32:Ao:226:UNK:O	32:Ao:229:UNK:HG3	1.75	0.86
46:BA:948:U:O4	46:BA:1377:C:N4	2.09	0.86
35:Az:702:UNK:O	35:Az:705:UNK:HG3	1.75	0.85
71:Bf:88:UNK:HG2	71:Bf:91:UNK:HG1	0.86	0.85
19:Aa:330:UNK:O	19:Aa:334:UNK:HG3	1.75	0.85
17:AV:8:Y5P:N3	17:AV:14:Y5P:H5	1.92	0.85
17:AY:32:Y5P:H4A	17:AY:33:Y5P:H4	1.59	0.85
19:Aa:310:UNK:HG3	19:Aa:313:UNK:CG	2.06	0.85
32:Ao:235:UNK:HG1	32:Ao:237:UNK:HB2	1.57	0.85
23:Ae:73:UNK:O	23:Ae:76:UNK:HG3	1.75	0.85
23:Ae:204:UNK:HB1	23:Ae:223:UNK:HG2	1.57	0.85
88:Bz:604:UNK:O	88:Bz:607:UNK:HG3	1.77	0.85
23:Ae:71:UNK:HA	23:Ae:74:UNK:HG3	1.58	0.85
23:Ae:163:UNK:HB2	23:Ae:184:UNK:HG1	1.57	0.85
49:BE:96:ARG:NH1	49:BE:301:ASP:OD2	2.09	0.85
38:B2:204:MET:HE2	38:B2:205:PRO:HD2	1.57	0.85
39:B3:119:ILE:H	83:Bt:45:ASN:HD21	1.23	0.85
64:BX:71:ARG:NH1	64:BX:96:TYR:OH	2.10	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:BF:83:HIS:HD2	50:BF:85:ASP:H	1.24	0.84
32:Ao:558:UNK:HG1	32:Ao:576:UNK:HG1	0.86	0.84
23:Ae:174:UNK:HG2	23:Ae:176:UNK:CG	1.99	0.84
23:Ae:217:UNK:HG2	23:Ae:252:UNK:HG3	1.57	0.84
2:AB:219:VAL:HG22	2:AB:233:TYR:HB2	1.60	0.84
41:B5:85:ARG:NH1	46:BA:640:G:OP1	2.11	0.84
23:Ae:67:UNK:O	23:Ae:100:UNK:HG1	1.77	0.84
23:Ae:181:UNK:HG2	23:Ae:210:UNK:CG	2.01	0.84
48:BD:115:GLU:OE1	48:BD:148:ARG:NH1	2.11	0.83
1:AA:576:C:HO2'	1:AA:809:G:HO2'	1.20	0.83
17:AV:42:Y5P:H4A	17:AV:43:Y5P:H4	1.59	0.83
23:Ae:273:UNK:HG2	23:Ae:276:UNK:CG	1.95	0.83
25:Ag:52:UNK:CG	25:Ag:66:UNK:HG3	2.08	0.83
54:BN:140:ASN:CB	73:Bh:262:GLY:HA2	2.08	0.83
17:AY:68:Y5P:H2'	17:AY:69:Y5P:H6	1.59	0.83
23:Ae:200:UNK:O	23:Ae:204:UNK:CG	2.20	0.83
32:Ao:341:UNK:O	32:Ao:344:UNK:HG3	1.77	0.83
23:Ae:247:UNK:O	23:Ae:247:UNK:HG2	1.76	0.83
32:Ao:191:UNK:HA	32:Ao:194:UNK:HG3	1.60	0.83
59:BS:107:THR:HG21	59:BS:119:THR:HG23	1.61	0.83
69:Bd:98:GLU:HA	75:Bj:83:LEU:HD11	1.61	0.83
86:Bw:97:THR:HG22	86:Bw:99:ALA:H	1.43	0.83
19:Aa:323:UNK:HG2	19:Aa:324:UNK:N	1.92	0.83
23:Ae:273:UNK:HG3	23:Ae:276:UNK:HG1	1.59	0.83
55:BO:72:ARG:HB2	55:BO:72:ARG:NH1	1.92	0.83
32:Ao:190:UNK:HG1	32:Ao:223:UNK:C	2.08	0.83
32:Ao:341:UNK:O	32:Ao:345:UNK:HG3	1.78	0.83
32:Ao:373:UNK:HG1	34:As:2363:UNK:HG3	1.61	0.83
33:Ap:95:ILE:HG22	33:Ap:100:VAL:HG22	1.61	0.83
88:Bz:421:UNK:HA	88:Bz:424:UNK:HG3	1.59	0.83
42:B6:26:THR:HG23	85:Bv:117:ARG:HH12	1.42	0.82
1:AA:209:C:H4'	13:AP:43:ARG:NH1	1.93	0.82
17:AV:37:Y5P:H4A	17:AV:38:Y5P:C4	2.09	0.82
23:Ae:104:UNK:CG	23:Ae:107:UNK:HG3	2.05	0.82
17:AY:23:Y5P:H4A	17:AY:24:Y5P:H4	1.59	0.82
19:Aa:325:UNK:O	19:Aa:329:UNK:HG3	1.79	0.82
68:Bc:140:TRP:HE1	68:Bc:171:VAL:HA	1.44	0.82
17:AY:55:Y5P:C5	17:AY:58:Y5P:H5	2.09	0.82
46:BA:68:A:O2'	46:BA:69:C:O4'	1.95	0.82
32:Ao:204:UNK:HA	32:Ao:207:UNK:HG3	1.59	0.82
58:BR:41:ARG:NH1	58:BR:134:LEU:HD13	1.94	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:Bf:88:UNK:O	71:Bf:91:UNK:CG	2.27	0.82
1:AA:475:A:OP2	5:AF:123:ARG:NH2	2.11	0.82
88:Bz:17:UNK:HA	88:Bz:20:UNK:HG3	1.61	0.82
14:AQ:13:VAL:HG23	14:AQ:66:LEU:HB2	1.61	0.82
23:Ae:251:UNK:O	23:Ae:255:UNK:HG3	1.80	0.82
35:Az:698:UNK:O	35:Az:701:UNK:HG3	1.80	0.82
61:BU:65:ARG:HH12	61:BU:99:ARG:NH1	1.76	0.82
17:AY:28:Y5P:H4A	17:AY:29:Y5P:H4	1.59	0.82
46:BA:134:G:O6	65:BY:34:LYS:NZ	2.11	0.82
19:Aa:326:UNK:O	19:Aa:330:UNK:CG	2.21	0.81
23:Ae:170:UNK:O	23:Ae:170:UNK:CG	2.24	0.81
1:AA:882:A:OP1	23:Ae:68:UNK:HG3	1.81	0.81
23:Ae:46:UNK:HG3	23:Ae:77:UNK:HG1	1.58	0.81
68:Bc:111:ASP:OD1	68:Bc:111:ASP:N	2.13	0.81
23:Ae:256:UNK:O	23:Ae:259:UNK:HG3	1.80	0.81
32:Ao:373:UNK:HG1	34:As:2360:UNK:HA	1.61	0.81
32:Ao:379:UNK:O	32:Ao:383:UNK:HG3	1.80	0.81
72:Bg:17:ASN:HD21	72:Bg:23:VAL:H	1.27	0.81
25:Ag:63:UNK:O	25:Ag:64:UNK:CG	2.28	0.81
46:BA:746:A:H8	86:Bw:308:GLN:HG2	1.43	0.81
79:Bn:69:HIS:HD2	79:Bn:71:LYS:H	1.28	0.81
6:AG:195:LYS:HB3	6:AG:204:LYS:HZ2	1.46	0.81
17:AV:55:Y5P:C1'	17:AV:57:Y5P:H5	2.10	0.81
17:AY:9:Y5P:H4A	17:AY:22:Y5P:H4A	1.59	0.81
32:Ao:497:UNK:O	32:Ao:500:UNK:HG3	1.81	0.81
23:Ae:208:UNK:CG	23:Ae:220:UNK:HG1	2.07	0.81
32:Ao:476:UNK:HB2	32:Ao:513:UNK:CG	2.11	0.81
23:Ae:233:UNK:C	23:Ae:236:UNK:HG3	2.11	0.81
71:Bf:92:UNK:O	71:Bf:95:UNK:CG	2.25	0.81
5:AF:9:ILE:HB	5:AF:89:ILE:HG22	1.63	0.81
23:Ae:174:UNK:HG1	23:Ae:176:UNK:HG3	1.53	0.80
23:Ae:299:UNK:O	23:Ae:303:UNK:HG3	1.81	0.80
41:B5:181:ARG:HH11	41:B5:187:GLN:HG2	1.44	0.80
23:Ae:301:UNK:HA	23:Ae:304:UNK:HG3	1.63	0.80
32:Ao:186:UNK:HG1	32:Ao:220:UNK:HB1	1.63	0.80
1:AA:103:G:OP1	14:AQ:78:LYS:NZ	2.13	0.80
32:Ao:521:UNK:HG1	32:Ao:534:UNK:HG1	1.62	0.80
50:BF:85:ASP:HB3	50:BF:274:LEU:HD21	1.61	0.80
4:AE:284:ARG:NH1	4:AE:328:GLY:O	2.14	0.80
17:AV:66:Y5P:H4A	17:AV:67:Y5P:H4	1.63	0.80
74:Bi:186:VAL:HG22	74:Bi:187:GLU:HG3	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Ae:34:UNK:O	23:Ae:37:UNK:HG3	1.82	0.80
28:Aj:121:LYS:HE3	28:Aj:123:LYS:NZ	1.97	0.80
73:Bh:105:ARG:HB2	73:Bh:112:LYS:HD2	1.63	0.80
17:AV:11:Y5P:H4A	17:AV:12:Y5P:H4	1.64	0.80
66:Ba:174:GLU:HA	66:Ba:296:SER:HB2	1.62	0.80
23:Ae:104:UNK:HG2	23:Ae:107:UNK:CG	2.07	0.80
32:Ao:190:UNK:CG	32:Ao:223:UNK:O	2.28	0.80
42:B6:38:ARG:NH2	46:BA:1185:U:OP2	2.15	0.80
92:AA:8113:HOH:O	17:AV:30:Y5P:H4A	1.81	0.80
1:AA:106:C:OP2	14:AQ:45:LYS:NZ	2.15	0.80
1:AA:491:G:OP1	31:An:135:ARG:NH2	2.13	0.80
19:Aa:310:UNK:CG	19:Aa:313:UNK:CG	2.60	0.80
23:Ae:108:UNK:O	23:Ae:111:UNK:HG3	1.81	0.79
32:Ao:196:UNK:HG2	32:Ao:206:UNK:HG1	1.61	0.79
46:BA:37:A:N6	70:Be:38:GLY:O	2.14	0.79
78:Bm:114:PRO:HG2	78:Bm:117:ARG:HG3	1.64	0.79
86:Bw:247:LEU:HD13	86:Bw:348:PRO:HG3	1.64	0.79
23:Ae:167:UNK:HG1	23:Ae:205:UNK:HG2	0.88	0.79
41:B5:81:PRO:HA	46:BA:1436:U:C2	2.17	0.79
17:AY:9:Y5P:H4A	17:AY:22:Y5P:C4	2.12	0.79
46:BA:442:G:O6	52:BJ:31:LYS:NZ	2.16	0.79
64:BX:50:ARG:NH1	64:BX:69:ARG:HA	1.95	0.79
1:AA:221:A:OP1	33:Ap:148:LYS:NZ	2.13	0.79
23:Ae:46:UNK:HG1	23:Ae:77:UNK:HG3	1.64	0.79
46:BA:996:C:OP1	92:BA:1852:HOH:O	2.00	0.79
23:Ae:163:UNK:HG3	23:Ae:206:UNK:HB2	1.64	0.79
16:AU:80:ARG:NH2	24:Af:165:GLU:OE2	2.15	0.79
23:Ae:118:UNK:CG	23:Ae:120:UNK:HG3	2.13	0.79
23:Ae:268:UNK:CG	33:Ap:214:SER:OG	2.30	0.79
32:Ao:359:UNK:HG2	32:Ao:396:UNK:CG	2.12	0.79
17:AV:59:Y5P:H4A	17:AV:60:Y5P:H4	1.63	0.79
23:Ae:181:UNK:CG	23:Ae:210:UNK:HG2	2.09	0.79
23:Ae:174:UNK:CG	23:Ae:176:UNK:HG2	2.10	0.79
46:BA:717:C:O2'	66:Ba:112:ARG:NH1	2.16	0.79
46:BA:911:G:O2'	46:BA:913:C:N4	2.15	0.79
46:BA:1043:U:H1'	49:BE:257:MET:HE3	1.64	0.79
69:Bd:83:ILE:HB	88:Bz:302:UNK:HB2	1.64	0.79
46:BA:778:G:OP2	86:Bw:219:ARG:NH2	2.14	0.79
47:BB:28:P5P:H2'	47:BB:29:P5P:H8	1.65	0.79
25:Ag:264:VAL:HG21	25:Ag:307:LEU:HB3	1.64	0.78
32:Ao:486:UNK:O	32:Ao:490:UNK:HG3	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:BF:205:GLU:HG2	50:BF:208:ARG:HH12	1.48	0.78
66:Ba:108:HIS:HD2	66:Ba:110:ARG:H	1.31	0.78
69:Bd:164:ARG:HH12	76:Bk:91:LEU:HD11	1.47	0.78
75:Bj:162:ARG:HH21	75:Bj:164:LYS:HE2	1.46	0.78
1:AA:707:A:H3'	1:AA:708:A:H5"	1.64	0.78
19:Aa:319:UNK:HG2	19:Aa:320:UNK:N	1.97	0.78
28:Aj:11:ILE:HG23	28:Aj:14:LEU:HD23	1.62	0.78
88:Bz:19:UNK:O	88:Bz:22:UNK:HG3	1.82	0.78
13:AP:93:LEU:O	19:Aa:174:ARG:NH1	2.16	0.78
23:Ae:114:UNK:HA	23:Ae:117:UNK:HG3	1.63	0.78
32:Ao:303:UNK:CG	32:Ao:340:UNK:HG2	2.14	0.78
45:B9:83:GLY:H	46:BA:1525:U:H5'	1.47	0.78
19:Aa:316:UNK:HB2	19:Aa:329:UNK:HG1	1.65	0.78
7:AI:260:UNK:HG3	7:AI:355:SER:HB3	1.66	0.78
23:Ae:38:UNK:O	23:Ae:41:UNK:HG3	1.84	0.78
23:Ae:176:UNK:O	23:Ae:180:UNK:HG2	1.84	0.78
32:Ao:318:UNK:O	32:Ao:322:UNK:HG3	1.84	0.78
52:BJ:103:ALA:HB3	81:Bp:39:SER:HA	1.66	0.78
1:AA:579:A:OP2	11:AN:96:ARG:NH1	2.15	0.78
1:AA:633:C:OP1	4:AE:269:ARG:NH1	2.17	0.78
23:Ae:170:UNK:HG1	28:Aj:78:ARG:HH22	1.49	0.78
30:Am:84:ARG:HG2	30:Am:87:ARG:NH1	1.99	0.78
32:Ao:160:UNK:HA	32:Ao:163:UNK:HG3	1.66	0.78
59:BS:86:THR:O	59:BS:120:ARG:NH1	2.17	0.78
66:Ba:144:ARG:O	66:Ba:194:LYS:NZ	2.16	0.78
86:Bw:213:ARG:HB2	86:Bw:213:ARG:NH1	1.98	0.78
23:Ae:391:UNK:C	23:Ae:394:UNK:HG3	2.14	0.78
47:BB:29:P5P:H2'	47:BB:30:P5P:H8	1.65	0.78
23:Ae:232:UNK:HG1	23:Ae:235:UNK:HG1	1.67	0.77
32:Ao:503:UNK:HB2	32:Ao:513:UNK:HG2	1.66	0.77
32:Ao:546:UNK:O	32:Ao:550:UNK:HG3	1.84	0.77
1:AA:103:G:H4'	14:AQ:8:VAL:HG13	1.66	0.77
36:B0:100:THR:HB	36:B0:132:HIS:HE2	1.48	0.77
39:B3:71:ARG:NH2	46:BA:472:G:OP1	2.17	0.77
23:Ae:63:UNK:CG	23:Ae:65:UNK:CG	2.59	0.77
23:Ae:147:UNK:O	23:Ae:151:UNK:HG2	1.85	0.77
23:Ae:127:UNK:O	23:Ae:131:UNK:HG3	1.84	0.77
23:Ae:356:UNK:O	23:Ae:360:UNK:HG3	1.84	0.77
48:BD:86:ASN:HD21	48:BD:90:GLN:HB2	1.50	0.77
71:Bf:87:UNK:CG	71:Bf:88:UNK:HG3	2.13	0.77
53:BK:43:GLY:HA3	53:BK:76:ARG:HH11	1.50	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:Ba:200:ARG:HH11	66:Ba:233:LYS:HD3	1.50	0.77
46:BA:497:C:O2	46:BA:548:A:N6	2.15	0.77
68:Bc:153:ARG:O	71:Bf:90:UNK:HG1	1.84	0.77
28:Aj:27:ARG:HH12	28:Aj:33:ARG:HH12	1.33	0.76
50:BF:287:ARG:HD2	85:Bv:33:ARG:HH12	1.50	0.76
84:Bu:166:UNK:O	84:Bu:167:UNK:HG3	1.85	0.76
68:Bc:294:GLN:HE22	68:Bc:320:VAL:H	1.30	0.76
28:Aj:95:TRP:HE1	28:Aj:131:ILE:HG12	1.49	0.76
38:B2:188:ILE:O	65:BY:216:TYR:OH	2.03	0.76
42:B6:38:ARG:HE	46:BA:1184:U:H3'	1.51	0.76
49:BE:68:GLU:OE1	68:Bc:311:LYS:NZ	2.16	0.76
52:BJ:162:LYS:HG3	52:BJ:195:SER:HB2	1.65	0.76
64:BX:44:ILE:HD12	64:BX:48:MET:HG2	1.68	0.76
46:BA:163:A:HO2'	46:BA:1014:C:H5	1.32	0.76
54:BN:156:ASP:OD1	54:BN:156:ASP:N	2.19	0.76
65:BY:163:ASP:O	74:Bi:71:ARG:NH1	2.18	0.76
17:AV:55:Y5P:O2'	17:AV:57:Y5P:H5	1.85	0.76
36:B0:50:ARG:NH1	46:BA:1198:A:OP1	2.17	0.76
73:Bh:259:ARG:HG3	73:Bh:259:ARG:NH1	1.95	0.76
23:Ae:197:UNK:HG1	23:Ae:230:UNK:CG	2.15	0.76
50:BF:74:GLN:O	50:BF:210:ARG:NH2	2.18	0.76
68:Bc:109:PRO:HB2	68:Bc:264:PRO:HG3	1.68	0.76
2:AB:79:SER:H	2:AB:82:SER:HB3	1.51	0.76
19:Aa:344:UNK:O	19:Aa:347:UNK:HG3	1.85	0.76
23:Ae:46:UNK:HG3	23:Ae:77:UNK:HG2	1.62	0.76
1:AA:437:C:OP1	9:AK:191:ARG:NH2	2.18	0.76
1:AA:631:A:H5'	3:AC:46:LYS:HE3	1.66	0.76
7:AI:253:UNK:CG	7:AI:366:ARG:HH12	1.98	0.75
19:Aa:319:UNK:HG2	19:Aa:320:UNK:H	1.49	0.75
88:Bz:28:UNK:HA	88:Bz:31:UNK:HG3	1.65	0.75
32:Ao:550:UNK:HA	32:Ao:553:UNK:HG3	1.67	0.75
46:BA:1481:C:H5'	49:BE:290:PRO:HA	1.68	0.75
17:AV:54:Y5P:C4	17:AV:58:Y5P:H5	2.15	0.75
64:BX:68:VAL:HG22	64:BX:97:VAL:HG12	1.67	0.75
71:Bf:51:LEU:HD13	71:Bf:58:ILE:HD13	1.68	0.75
2:AB:109:ARG:NH1	20:Ab:68:ASP:OD2	2.18	0.75
46:BA:529:G:O2'	82:Bq:127:TRP:NE1	2.17	0.75
66:Ba:347:THR:HG22	66:Ba:349:GLY:H	1.51	0.75
27:Ai:13:ARG:NH2	35:Az:692:UNK:HG2	2.01	0.75
55:BO:74:LEU:HD11	55:BO:81:LYS:HB3	1.69	0.75
1:AA:566:U:O2	1:AA:686:A:N6	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Ae:207:UNK:CG	23:Ae:219:UNK:HG2	2.16	0.75
46:BA:170:A:OP1	71:Bf:135:LYS:NZ	2.17	0.75
50:BF:262:THR:HG22	50:BF:264:PRO:HD2	1.69	0.75
66:Ba:140:ALA:HB1	66:Ba:412:ARG:HG2	1.69	0.75
33:Ap:95:ILE:HG13	33:Ap:145:LYS:HZ3	1.51	0.75
46:BA:276:A:H2'	46:BA:277:A:H5"	1.68	0.75
64:BX:69:ARG:NH1	86:Bw:266:PRO:HD3	2.02	0.75
32:Ao:225:UNK:O	32:Ao:228:UNK:HG3	1.87	0.75
40:B4:58:VAL:HG22	40:B4:64:THR:HG22	1.66	0.75
17:AY:55:Y5P:H6	17:AY:57:Y5P:H5	1.67	0.74
19:Aa:89:ILE:O	19:Aa:124:ARG:NH1	2.20	0.74
25:Ag:55:UNK:HG2	25:Ag:56:UNK:N	1.99	0.74
49:BE:113:ASP:N	49:BE:113:ASP:OD1	2.18	0.74
50:BF:59:ARG:HG2	50:BF:59:ARG:NH1	1.97	0.74
58:BR:143:LEU:HB3	68:Bc:132:PRO:HD2	1.68	0.74
23:Ae:232:UNK:CG	23:Ae:235:UNK:CG	2.65	0.74
52:BJ:161:VAL:HG21	52:BJ:194:TYR:HB3	1.69	0.74
32:Ao:339:UNK:O	32:Ao:342:UNK:HG3	1.87	0.74
8:AJ:128:LYS:HG2	8:AJ:131:ARG:HH21	1.50	0.74
32:Ao:427:UNK:HG2	32:Ao:466:UNK:HG1	1.69	0.74
66:Ba:147:ILE:H	66:Ba:150:GLN:HE21	1.33	0.74
1:AA:458:C:O2'	1:AA:460:A:OP2	2.05	0.74
23:Ae:118:UNK:HG2	23:Ae:120:UNK:HG3	1.68	0.74
61:BU:94:GLN:HB2	62:BV:150:LYS:HG2	1.70	0.74
17:AV:24:Y5P:H4A	17:AV:25:Y5P:H4	1.69	0.74
22:Ad:59:ARG:NH1	33:Ap:202:TRP:O	2.20	0.74
85:Bv:41:ASP:HB2	85:Bv:44:ASP:HB2	1.69	0.74
32:Ao:306:UNK:HG1	32:Ao:320:UNK:HB2	1.70	0.74
32:Ao:671:UNK:HA	32:Ao:674:UNK:HG3	1.68	0.74
17:AY:67:Y5P:H4A	17:AY:68:Y5P:H4	1.68	0.74
46:BA:163:A:OP2	61:BU:48:ARG:NH1	2.20	0.74
46:BA:293:G:H5'	63:BW:159:ARG:HD2	1.68	0.74
26:Ah:371:TYR:OH	26:Ah:375:LYS:NZ	2.20	0.74
84:Bu:167:UNK:O	84:Bu:167:UNK:HG2	1.86	0.74
5:AF:79:MET:HE1	5:AF:92:ASN:HA	1.70	0.74
32:Ao:189:UNK:HA	32:Ao:192:UNK:HG3	1.70	0.74
46:BA:162:C:H5	46:BA:1011:A:H61	1.36	0.74
72:Bg:28:ARG:HH21	73:Bh:177:GLN:HE21	1.36	0.74
88:Bz:26:UNK:O	88:Bz:29:UNK:HG3	1.87	0.74
7:AI:228:ARG:HD2	16:AU:85:GLN:HE21	1.51	0.73
56:BP:14:ASP:OD1	56:BP:17:ARG:NH1	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:Bc:273:PHE:HD2	68:Bc:274:GLN:HG3	1.53	0.73
86:Bw:146:GLN:HE21	86:Bw:151:LEU:HD22	1.53	0.73
5:AF:3:ARG:NH1	5:AF:4:TYR:HE1	1.86	0.73
88:Bz:24:UNK:C	88:Bz:27:UNK:HG3	2.17	0.73
1:AA:361:A:N6	92:AA:8120:HOH:O	2.16	0.73
9:AK:160:ARG:NH1	16:AU:23:TYR:OH	2.21	0.73
23:Ae:179:UNK:HG3	23:Ae:362:UNK:HB2	1.69	0.73
66:Ba:153:ARG:NH2	86:Bw:191:ALA:HA	2.00	0.73
88:Bz:20:UNK:O	88:Bz:23:UNK:HG3	1.87	0.73
88:Bz:21:UNK:HA	88:Bz:24:UNK:HG3	1.70	0.73
52:BJ:148:VAL:HG11	81:Bp:28:GLU:HG2	1.70	0.73
19:Aa:343:UNK:C	19:Aa:346:UNK:HG3	2.17	0.73
23:Ae:188:UNK:O	23:Ae:192:UNK:CG	2.36	0.73
7:AI:382:LYS:NZ	7:AI:388:ALA:O	2.16	0.73
32:Ao:480:UNK:O	32:Ao:483:UNK:HG3	1.88	0.73
32:Ao:538:UNK:HG2	32:Ao:550:UNK:HB2	1.70	0.73
32:Ao:581:UNK:CG	32:Ao:654:UNK:HG2	2.15	0.73
47:BB:28:P5P:H4'	69:Bd:133:ARG:HH12	1.53	0.73
65:BY:130:PRO:O	65:BY:149:ARG:NH1	2.22	0.73
19:Aa:317:UNK:HG2	19:Aa:318:UNK:N	2.02	0.73
48:BD:136:ARG:HG2	48:BD:136:ARG:HH11	1.53	0.73
73:Bh:60:ARG:HH11	73:Bh:63:LYS:HB2	1.52	0.73
88:Bz:31:UNK:C	88:Bz:34:UNK:HG3	2.18	0.73
4:AE:160:ARG:NH1	4:AE:165:GLN:OE1	2.21	0.73
29:Ak:166:ARG:HB2	32:Ao:134:GLU:HG3	1.69	0.73
32:Ao:157:UNK:CG	32:Ao:173:UNK:HG2	2.17	0.73
46:BA:658:C:H4'	58:BR:81:THR:HG21	1.69	0.73
1:AA:12:G:H5'	4:AE:229:PHE:HD2	1.52	0.73
6:AG:64:TYR:HA	6:AG:67:ASP:HB2	1.70	0.73
32:Ao:241:UNK:HA	32:Ao:244:UNK:HG3	1.70	0.73
54:BN:27:PRO:HG2	54:BN:30:LYS:HB2	1.70	0.73
54:BN:114:LYS:HA	54:BN:118:ARG:NH1	2.04	0.73
11:AN:41:ARG:HD3	11:AN:87:ILE:HD13	1.70	0.73
20:Ab:30:LEU:H	20:Ab:30:LEU:HD12	1.53	0.73
26:Ah:351:SER:OG	29:Ak:213:ARG:NH1	2.21	0.73
32:Ao:194:UNK:CA	32:Ao:230:UNK:HG1	2.16	0.73
52:BJ:93:ASN:HD22	52:BJ:96:ILE:HG12	1.53	0.73
57:BQ:209:ASN:ND2	57:BQ:211:ASN:OD1	2.21	0.73
9:AK:65:TYR:HB3	16:AU:13:MET:H	1.53	0.72
32:Ao:554:UNK:HG3	32:Ao:576:UNK:HB2	1.70	0.72
1:AA:858:C:H42	1:AA:912:A:H61	1.36	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Aa:324:UNK:O	19:Aa:328:UNK:CG	2.25	0.72
25:Ag:209:TRP:HZ3	25:Ag:215:THR:HB	1.55	0.72
32:Ao:366:UNK:HG1	32:Ao:400:UNK:HG2	1.70	0.72
46:BA:213:A:O3'	50:BF:92:ARG:NH2	2.21	0.72
1:AA:56:U:O2'	1:AA:198:C:O2	2.08	0.72
19:Aa:300:VAL:CG1	19:Aa:330:UNK:HG1	2.19	0.72
23:Ae:298:UNK:HA	23:Ae:301:UNK:HG3	1.71	0.72
48:BD:258:ILE:HG23	48:BD:263:ARG:HB3	1.71	0.72
62:BV:159:ARG:NH1	62:BV:161:GLU:OE2	2.22	0.72
1:AA:744:C:H3'	1:AA:745:C:H4'	1.71	0.72
17:AV:67:Y5P:H4A	17:AV:68:Y5P:H4	1.70	0.72
32:Ao:82:SER:O	32:Ao:446:UNK:HG1	1.89	0.72
46:BA:786:A:C5	58:BR:17:ARG:HD2	2.24	0.72
19:Aa:311:UNK:CG	19:Aa:312:UNK:N	2.52	0.72
23:Ae:70:UNK:C	23:Ae:73:UNK:HG3	2.18	0.72
26:Ah:301:LYS:HG2	32:Ao:137:ILE:HG21	1.71	0.72
50:BF:292:ASP:OD1	50:BF:292:ASP:N	2.22	0.72
86:Bw:91:TYR:HB3	86:Bw:267:LEU:HD13	1.71	0.72
19:Aa:189:ASP:OD1	19:Aa:201:ARG:NH1	2.22	0.72
21:Ac:78:PHE:HB2	21:Ac:86:VAL:HB	1.70	0.72
23:Ae:93:UNK:O	23:Ae:97:UNK:HG3	1.90	0.72
29:Ak:154:ASP:HB2	29:Ak:174:THR:HB	1.71	0.72
44:B8:137:THR:HG22	44:B8:139:ALA:H	1.54	0.72
73:Bh:265:THR:HG22	73:Bh:267:LEU:H	1.54	0.72
23:Ae:286:UNK:O	23:Ae:289:UNK:HG3	1.90	0.72
54:BN:114:LYS:HA	54:BN:118:ARG:HH12	1.54	0.72
65:BY:133:VAL:HG13	65:BY:145:ARG:HB3	1.72	0.72
31:An:144:ARG:HH12	31:An:147:VAL:HG11	1.54	0.72
32:Ao:486:UNK:O	32:Ao:490:UNK:CG	2.38	0.72
33:Ap:73:VAL:HG12	33:Ap:106:PRO:HB2	1.72	0.72
23:Ae:200:UNK:CG	23:Ae:226:UNK:HG1	2.20	0.72
33:Ap:59:LEU:HD13	33:Ap:121:LYS:HB2	1.72	0.72
88:Bz:399:UNK:O	88:Bz:402:UNK:HG3	1.89	0.72
29:Ak:189:LYS:HD3	29:Ak:190:LYS:HG3	1.72	0.71
47:BB:62:Y5P:H4A	47:BB:63:Y5P:H4	1.72	0.71
66:Ba:160:HIS:HA	66:Ba:164:TRP:HB2	1.72	0.71
69:Bd:100:GLN:HG2	75:Bj:84:TYR:HA	1.71	0.71
75:Bj:265:LYS:HG3	75:Bj:266:PRO:HD3	1.72	0.71
19:Aa:315:UNK:HG2	19:Aa:316:UNK:N	2.05	0.71
23:Ae:175:UNK:CG	23:Ae:368:UNK:HG3	2.20	0.71
32:Ao:394:UNK:HA	32:Ao:397:UNK:HG3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:B5:130:VAL:HG21	58:BR:135:PRO:HD3	1.72	0.71
46:BA:598:C:H5"	56:BP:50:GLY:HA2	1.72	0.71
46:BA:723:C:H5	66:Ba:389:LEU:H	1.39	0.71
23:Ae:390:UNK:O	23:Ae:393:UNK:HG3	1.89	0.71
32:Ao:558:UNK:HG3	32:Ao:576:UNK:HG1	1.71	0.71
88:Bz:405:UNK:C	88:Bz:408:UNK:HG3	2.19	0.71
14:AQ:95:VAL:HG11	22:Ad:120:ARG:HH22	1.55	0.71
28:Aj:87:TRP:O	33:Ap:215:ARG:NE	2.23	0.71
46:BA:1048:C:H2'	46:BA:1325:U:H4'	1.71	0.71
50:BF:167:MET:HA	50:BF:170:ARG:HH21	1.55	0.71
52:BJ:95:MET:HE2	52:BJ:159:PRO:HB2	1.73	0.71
56:BP:130:GLN:NE2	92:BP:401:HOH:O	2.23	0.71
1:AA:645:A:H5'	1:AA:646:C:H5	1.55	0.71
4:AE:191:ARG:NH2	33:Ap:80:ASN:OD1	2.24	0.71
16:AU:49:CYS:SG	16:AU:50:ARG:N	2.63	0.71
17:AY:30:Y5P:H4A	17:AY:31:Y5P:H4	1.71	0.71
19:Aa:182:LYS:HZ3	33:Ap:183:ALA:HA	1.56	0.71
23:Ae:232:UNK:CG	23:Ae:235:UNK:HG1	2.20	0.71
23:Ae:388:UNK:O	23:Ae:392:UNK:HG3	1.91	0.71
46:BA:684:C:OP2	92:BA:1930:HOH:O	2.08	0.71
1:AA:811:U:H5'	8:AJ:131:ARG:HH12	1.55	0.71
58:BR:41:ARG:HB2	58:BR:125:GLU:HG3	1.73	0.71
1:AA:606:A:HO2'	11:AN:28:TYR:HH	1.37	0.71
23:Ae:120:UNK:O	23:Ae:124:UNK:HG3	1.89	0.71
17:AY:55:Y5P:C6	17:AY:58:Y5P:H5	2.19	0.71
32:Ao:196:UNK:HG1	32:Ao:206:UNK:HG1	1.73	0.71
46:BA:746:A:C8	86:Bw:308:GLN:HG2	2.25	0.71
59:BS:88:HIS:HB3	59:BS:89:HIS:HD2	1.55	0.71
64:BX:45:PRO:HD2	64:BX:48:MET:HE2	1.73	0.71
1:AA:361:A:OP1	5:AF:57:ARG:NH1	2.24	0.71
26:Ah:326:LEU:HB2	26:Ah:347:THR:HG23	1.73	0.71
29:Ak:246:THR:HG22	29:Ak:248:ALA:H	1.53	0.71
32:Ao:539:UNK:HG2	32:Ao:551:UNK:HB1	1.72	0.71
46:BA:819:C:O2'	46:BA:951:G:OP1	2.09	0.71
1:AA:512:A:H2'	1:AA:513:A:H8	1.56	0.71
23:Ae:243:UNK:O	23:Ae:244:UNK:HG3	1.91	0.71
23:Ae:267:UNK:CG	23:Ae:270:UNK:HG3	2.21	0.71
25:Ag:54:UNK:HG1	25:Ag:67:UNK:HA	1.73	0.71
46:BA:741:U:H3'	46:BA:742:A:H5"	1.73	0.71
46:BA:875:U:O2'	46:BA:963:A:OP2	2.08	0.71
50:BF:205:GLU:HG2	50:BF:208:ARG:NH1	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:Bd:97:LYS:HA	69:Bd:99:ARG:NH1	2.05	0.71
23:Ae:139:UNK:CG	23:Ae:140:UNK:N	2.54	0.70
46:BA:1517:U:OP1	87:Bx:94:ARG:NH2	2.24	0.70
1:AA:648:A:OP1	2:AB:200:ASN:ND2	2.24	0.70
23:Ae:170:UNK:HG1	28:Aj:78:ARG:NH2	2.06	0.70
32:Ao:653:UNK:HA	32:Ao:656:UNK:HG3	1.74	0.70
46:BA:705:A:N1	86:Bw:97:THR:HG23	2.06	0.70
1:AA:670:A:N3	6:AG:36:ARG:NH1	2.40	0.70
62:BV:102:VAL:HB	62:BV:139:LEU:HB3	1.72	0.70
88:Bz:602:UNK:O	88:Bz:606:UNK:HG3	1.91	0.70
88:Bz:610:UNK:HA	88:Bz:613:UNK:HG3	1.73	0.70
17:AY:3:Y5P:H4A	17:AY:4:Y5P:H4	1.71	0.70
19:Aa:309:UNK:O	19:Aa:309:UNK:HG2	1.92	0.70
23:Ae:124:UNK:O	23:Ae:127:UNK:HG3	1.91	0.70
32:Ao:264:UNK:HB2	32:Ao:289:UNK:HG3	1.73	0.70
52:BJ:63:ARG:NH1	87:Bx:108:CYS:HA	2.06	0.70
75:Bj:187:THR:HG23	75:Bj:190:ARG:HH21	1.56	0.70
61:BU:112:THR:H	72:Bg:127:GLN:HE22	1.40	0.70
66:Ba:144:ARG:HB3	66:Ba:194:LYS:HZ1	1.57	0.70
79:Bn:45:ASP:O	79:Bn:51:ARG:NH1	2.25	0.70
1:AA:117:C:OP1	31:An:175:ARG:NH1	2.24	0.70
50:BF:211:ARG:NH2	78:Bm:57:GLN:O	2.23	0.70
88:Bz:606:UNK:HA	88:Bz:609:UNK:HG3	1.74	0.70
2:AB:93:LYS:HE2	24:Af:149:GLU:HG2	1.73	0.70
32:Ao:358:UNK:O	32:Ao:362:UNK:HG3	1.92	0.70
32:Ao:373:UNK:CG	34:As:2363:UNK:HG3	2.17	0.70
32:Ao:655:UNK:O	32:Ao:659:UNK:HG3	1.92	0.70
23:Ae:173:UNK:HG2	23:Ae:173:UNK:O	1.89	0.70
25:Ag:259:VAL:HG11	25:Ag:295:MET:HG3	1.73	0.70
46:BA:618:A:O2'	46:BA:619:U:H6	1.72	0.70
3:AC:52:THR:HG22	3:AC:54:GLU:H	1.56	0.70
4:AE:198:TRP:HB2	4:AE:225:VAL:HG11	1.74	0.70
42:B6:37:LEU:HD11	42:B6:40:LYS:HG3	1.74	0.70
46:BA:512:A:O2'	46:BA:513:A:OP2	2.08	0.70
46:BA:1250:G:N7	92:BA:1842:HOH:O	2.24	0.70
49:BE:165:TYR:CE2	49:BE:172:PRO:HA	2.27	0.70
56:BP:104:LEU:HD11	56:BP:126:GLY:HA3	1.73	0.70
71:Bf:84:UNK:HA	71:Bf:92:UNK:HB2	1.73	0.70
5:AF:90:ARG:NH1	15:AR:117:ILE:O	2.25	0.70
11:AN:60:ASN:O	11:AN:68:GLN:NE2	2.24	0.70
23:Ae:68:UNK:CG	23:Ae:71:UNK:HG3	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:BD:64:VAL:O	48:BD:80:ARG:NH2	2.21	0.70
88:Bz:29:UNK:O	88:Bz:33:UNK:HG3	1.92	0.70
17:AY:6:Y5P:C4	17:AY:7:Y5P:H4	2.17	0.69
23:Ae:48:UNK:HB2	23:Ae:53:UNK:HG2	1.74	0.69
29:Ak:88:ARG:HB3	29:Ak:98:PRO:HB2	1.72	0.69
35:Az:693:UNK:HG2	35:Az:693:UNK:O	1.92	0.69
60:BT:66:UNK:O	60:BT:66:UNK:CG	2.39	0.69
1:AA:647:A:H1'	2:AB:148:ARG:NH1	2.07	0.69
19:Aa:312:UNK:O	19:Aa:316:UNK:CG	2.31	0.69
19:Aa:322:UNK:O	19:Aa:326:UNK:HG3	1.92	0.69
46:BA:428:G:OP1	56:BP:62:ARG:NH2	2.25	0.69
52:BJ:156:SER:HB3	52:BJ:159:PRO:HB3	1.74	0.69
32:Ao:303:UNK:HG2	32:Ao:340:UNK:HG2	1.73	0.69
37:B1:5:LYS:HG3	37:B1:6:VAL:HG12	1.73	0.69
55:BO:73:ILE:HG22	55:BO:84:ALA:HB3	1.74	0.69
85:Bv:142:ARG:O	85:Bv:145:UNK:HG3	1.92	0.69
17:AY:27:Y5P:O5'	17:AY:27:Y5P:H6	1.90	0.69
23:Ae:267:UNK:HB1	33:Ap:218:ARG:HD3	1.73	0.69
32:Ao:359:UNK:CG	32:Ao:396:UNK:CG	2.69	0.69
32:Ao:442:UNK:O	32:Ao:446:UNK:HG3	1.92	0.69
45:B9:100:MET:HE2	46:BA:559:C:H1'	1.74	0.69
81:Bp:8:LEU:HD13	81:Bp:95:GLN:HG3	1.72	0.69
19:Aa:70:MET:HA	19:Aa:75:GLN:HE21	1.56	0.69
23:Ae:84:UNK:CG	23:Ae:86:UNK:HG3	2.22	0.69
46:BA:1264:U:H2'	46:BA:1265:A:H8	1.57	0.69
57:BQ:118:MET:HE2	57:BQ:163:MET:HE1	1.73	0.69
1:AA:588:A:OP1	11:AN:33:LYS:NZ	2.26	0.69
1:AA:882:A:OP1	23:Ae:68:UNK:HG1	1.92	0.69
17:AY:36:P5P:H2'	17:AY:37:Y5P:H6	1.73	0.69
32:Ao:245:UNK:HA	32:Ao:248:UNK:HG3	1.75	0.69
48:BD:69:ARG:HH11	48:BD:69:ARG:HB2	1.57	0.69
87:Bx:99:MET:HE3	87:Bx:116:GLU:HA	1.74	0.69
19:Aa:330:UNK:O	19:Aa:334:UNK:CG	2.41	0.69
32:Ao:232:UNK:CB	32:Ao:241:UNK:HG1	2.23	0.69
38:B2:175:PHE:O	38:B2:214:ARG:NH2	2.25	0.69
61:BU:65:ARG:HH12	61:BU:99:ARG:HH11	1.39	0.69
78:Bm:74:HIS:HA	78:Bm:77:GLU:HG2	1.74	0.69
1:AA:512:A:H2'	1:AA:513:A:C8	2.28	0.69
10:AL:32:THR:HG23	10:AL:35:GLN:HE21	1.57	0.69
17:AY:14:Y5P:H4A	17:AY:15:Y5P:H4	1.75	0.69
20:Ab:93:LYS:HD3	20:Ab:97:GLN:HG2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Ae:398:UNK:HA	23:Ae:401:UNK:HG3	1.73	0.69
30:Am:11:ALA:HB2	30:Am:19:PRO:HG3	1.74	0.69
32:Ao:242:UNK:HA	32:Ao:245:UNK:HG3	1.75	0.69
46:BA:567:C:H5'	87:Bx:166:GLY:H	1.57	0.69
60:BT:99:MET:HB2	60:BT:167:TYR:CE1	2.28	0.69
66:Ba:213:TRP:HE1	66:Ba:215:ARG:HB2	1.57	0.69
68:Bc:187:ASP:HA	68:Bc:291:ARG:HH22	1.56	0.69
74:Bi:80:CYS:SG	74:Bi:165:THR:OG1	2.43	0.69
19:Aa:316:UNK:HB2	19:Aa:329:UNK:CG	2.23	0.69
23:Ae:221:UNK:HA	23:Ae:224:UNK:HG3	1.74	0.69
45:B9:65:THR:HG23	45:B9:100:MET:HB3	1.75	0.69
56:BP:28:LYS:NZ	56:BP:31:PRO:HD3	2.07	0.69
66:Ba:313:MET:HE1	66:Ba:346:GLY:HA3	1.73	0.69
71:Bf:95:UNK:O	71:Bf:98:UNK:HG3	1.93	0.69
69:Bd:157:LEU:HD13	75:Bj:232:PHE:HE2	1.56	0.69
46:BA:529:G:H1	46:BA:544:C:H42	1.40	0.68
67:Bb:157:LEU:HD13	67:Bb:221:LEU:HD11	1.74	0.68
88:Bz:606:UNK:O	88:Bz:609:UNK:HG3	1.92	0.68
10:AL:69:LYS:NZ	10:AL:77:ASN:HB3	2.07	0.68
17:AY:38:Y5P:H4A	17:AY:39:Y5P:H4	1.75	0.68
32:Ao:339:UNK:CG	32:Ao:376:UNK:HB1	2.18	0.68
35:Az:703:UNK:O	35:Az:707:UNK:CG	2.37	0.68
37:B1:96:LYS:O	46:BA:60:U:O2'	2.11	0.68
46:BA:147:A:H4'	46:BA:148:A:H5"	1.75	0.68
46:BA:417:U:OP1	80:Bo:76:ARG:NH2	2.20	0.68
50:BF:92:ARG:NH1	50:BF:95:ILE:HD11	2.09	0.68
50:BF:174:LEU:HD23	50:BF:253:MET:HE1	1.74	0.68
19:Aa:96:GLU:HA	33:Ap:131:THR:HG23	1.75	0.68
23:Ae:232:UNK:HG2	23:Ae:235:UNK:HG3	1.73	0.68
46:BA:136:A:H5"	65:BY:85:TRP:CH2	2.29	0.68
60:BT:192:ASP:OD2	60:BT:233:TRP:NE1	2.18	0.68
66:Ba:153:ARG:HH11	66:Ba:187:LEU:HD22	1.58	0.68
66:Ba:192:ILE:HG13	66:Ba:198:LEU:HB2	1.73	0.68
71:Bf:78:UNK:O	71:Bf:78:UNK:HG2	1.92	0.68
1:AA:826:C:H2'	1:AA:827:A:H8	1.58	0.68
10:AL:55:ARG:HD3	10:AL:58:LEU:HD21	1.76	0.68
23:Ae:51:UNK:O	23:Ae:55:UNK:HG2	1.92	0.68
23:Ae:246:UNK:O	23:Ae:247:UNK:HG3	1.93	0.68
23:Ae:296:UNK:HA	23:Ae:299:UNK:HG3	1.74	0.68
32:Ao:478:UNK:HA	32:Ao:481:UNK:HG3	1.75	0.68
32:Ao:521:UNK:CG	32:Ao:534:UNK:HG1	2.22	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:BA:973:G:O2'	46:BA:975:G:OP2	2.11	0.68
61:BU:112:THR:H	72:Bg:127:GLN:NE2	1.91	0.68
2:AB:57:LEU:HB2	2:AB:270:TYR:HE2	1.58	0.68
17:AV:62:Y5P:H4A	17:AV:63:Y5P:H4	1.75	0.68
40:B4:61:ASP:HB3	40:B4:63:SER:H	1.57	0.68
50:BF:283:LEU:HB2	56:BP:125:ARG:HH12	1.59	0.68
65:BY:170:TRP:O	70:Be:75:ARG:NH2	2.27	0.68
77:Bl:96:VAL:HG22	77:Bl:110:ILE:HG12	1.74	0.68
27:Ai:17:ARG:NH2	35:Az:698:UNK:CG	2.51	0.68
32:Ao:521:UNK:CB	32:Ao:534:UNK:HG1	2.23	0.68
35:Az:702:UNK:O	35:Az:706:UNK:HG3	1.94	0.68
46:BA:1416:G:N2	46:BA:1419:A:OP2	2.25	0.68
70:Be:16:ASP:HB3	70:Be:25:ARG:HH22	1.58	0.68
75:Bj:255:VAL:HG13	75:Bj:259:GLU:HB2	1.76	0.68
4:AE:160:ARG:HD2	4:AE:165:GLN:HE22	1.57	0.68
23:Ae:134:UNK:O	23:Ae:135:UNK:CG	2.37	0.68
32:Ao:228:UNK:HA	32:Ao:231:UNK:HG3	1.75	0.68
32:Ao:396:UNK:C	32:Ao:399:UNK:HG3	2.22	0.68
39:B3:114:LYS:NZ	83:Bt:46:GLN:OE1	2.26	0.68
41:B5:93:ARG:NH1	46:BA:642:G:OP2	2.27	0.68
50:BF:279:ARG:NH1	50:BF:286:PHE:HE2	1.92	0.68
1:AA:702:G:H5'	11:AN:36:ARG:HD3	1.74	0.68
23:Ae:31:UNK:O	23:Ae:35:UNK:HG3	1.94	0.68
54:BN:15:ALA:HB1	73:Bh:269:VAL:HG21	1.74	0.68
60:BT:246:ASP:OD1	60:BT:246:ASP:N	2.26	0.68
64:BX:28:LEU:HD11	64:BX:40:VAL:HG12	1.76	0.68
76:Bk:94:HIS:HB2	76:Bk:185:SER:HB3	1.76	0.68
84:Bu:75:ARG:NH1	84:Bu:108:ASP:OD1	2.26	0.68
19:Aa:319:UNK:CG	19:Aa:320:UNK:H	2.06	0.68
23:Ae:217:UNK:HG2	23:Ae:252:UNK:CG	2.23	0.68
41:B5:156:THR:HG21	41:B5:173:ARG:NH1	2.08	0.68
67:Bb:47:ARG:HG3	76:Bk:120:LYS:HZ3	1.59	0.68
75:Bj:159:LEU:HD23	75:Bj:174:PRO:HG3	1.75	0.68
7:AI:274:GLU:HG2	7:AI:283:GLU:HG2	1.75	0.68
14:AQ:69:LEU:HD12	14:AQ:70:PRO:HD2	1.76	0.68
35:Az:701:UNK:HG2	35:Az:702:UNK:N	2.08	0.68
48:BD:202:GLY:O	66:Ba:30:ALA:N	2.27	0.68
17:AV:64:Y5P:H4A	17:AV:65:Y5P:H4	1.76	0.67
21:Ac:35:ASN:OD1	21:Ac:69:ASN:ND2	2.27	0.67
32:Ao:306:UNK:CG	32:Ao:320:UNK:HB2	2.25	0.67
73:Bh:202:LEU:HD23	73:Bh:211:THR:HG23	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AV:4:Y5P:H4A	17:AV:5:Y5P:H4	1.74	0.67
23:Ae:400:UNK:C	23:Ae:403:UNK:HG3	2.24	0.67
32:Ao:533:UNK:O	32:Ao:536:UNK:HG3	1.95	0.67
6:AG:71:THR:HA	7:AI:253:UNK:HG1	1.76	0.67
7:AI:111:LEU:HD22	29:Ak:114:LEU:HD23	1.74	0.67
29:Ak:252:GLU:HA	29:Ak:303:ASN:HD21	1.60	0.67
32:Ao:482:UNK:HA	32:Ao:485:UNK:HG3	1.76	0.67
17:AV:55:Y5P:HC	17:AV:57:Y5P:H5	1.76	0.67
20:Ab:67:GLU:HA	20:Ab:70:ILE:HD12	1.77	0.67
23:Ae:232:UNK:HG2	23:Ae:235:UNK:CG	2.24	0.67
32:Ao:355:UNK:O	32:Ao:358:UNK:HG3	1.95	0.67
36:B0:124:ALA:O	67:Bb:51:TYR:OH	2.10	0.67
41:B5:181:ARG:NH1	41:B5:187:GLN:HA	2.10	0.67
54:BN:65:ILE:HD11	54:BN:104:VAL:HG23	1.76	0.67
72:Bg:35:ARG:HB2	83:Bt:101:TRP:HB2	1.76	0.67
23:Ae:51:UNK:HB1	60:BT:65:UNK:HB1	1.76	0.67
25:Ag:265:ASN:OD1	25:Ag:265:ASN:N	2.25	0.67
46:BA:68:A:O2'	46:BA:69:C:O5'	2.12	0.67
46:BA:925:A:H2'	46:BA:926:G:O4'	1.94	0.67
72:Bg:28:ARG:NH1	73:Bh:71:GLU:OE2	2.27	0.67
19:Aa:342:UNK:HA	19:Aa:345:UNK:HG3	1.77	0.67
32:Ao:373:UNK:HG2	32:Ao:374:UNK:N	2.08	0.67
50:BF:111:TYR:HE2	79:Bn:77:PRO:HD3	1.59	0.67
71:Bf:126:ARG:HG2	71:Bf:126:ARG:HH11	1.59	0.67
86:Bw:369:ASN:H	86:Bw:385:ASN:HD22	1.42	0.67
1:AA:835:C:H2'	1:AA:836:G:C8	2.30	0.67
19:Aa:350:UNK:C	19:Aa:353:UNK:HG3	2.24	0.67
23:Ae:288:UNK:O	23:Ae:291:UNK:HG3	1.94	0.67
38:B2:80:LYS:HZ3	74:Bi:71:ARG:HE	1.43	0.67
46:BA:616:A:OP2	79:Bn:41:ARG:NH1	2.28	0.67
60:BT:233:TRP:HB3	60:BT:240:ILE:HD12	1.75	0.67
65:BY:18:ASN:OD1	65:BY:43:ARG:NH1	2.28	0.67
69:Bd:164:ARG:NH1	76:Bk:88:TYR:HB3	2.10	0.67
71:Bf:87:UNK:CG	71:Bf:88:UNK:N	2.57	0.67
11:AN:58:ARG:HB3	11:AN:58:ARG:HH11	1.59	0.67
32:Ao:413:UNK:HA	32:Ao:416:UNK:HG3	1.77	0.67
37:B1:96:LYS:NZ	46:BA:82:G:OP1	2.27	0.67
71:Bf:74:PRO:HA	73:Bh:256:ARG:HD2	1.76	0.67
77:Bl:140:VAL:H	83:Bt:85:HIS:CD2	2.12	0.67
6:AG:85:VAL:HG22	25:Ag:369:LYS:HD3	1.77	0.67
7:AI:253:UNK:HG3	7:AI:366:ARG:NH1	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Ae:134:UNK:C	23:Ae:135:UNK:HG3	2.25	0.67
41:B5:152:PRO:HG3	41:B5:173:ARG:HH11	1.59	0.67
71:Bf:87:UNK:HG2	71:Bf:88:UNK:N	2.09	0.67
81:Bp:18:VAL:HG13	81:Bp:64:VAL:HG22	1.77	0.67
86:Bw:251:ILE:HG22	86:Bw:253:ILE:H	1.58	0.67
17:AV:51:Y5P:H2'	17:AV:52:Y5P:C6	2.25	0.67
23:Ae:280:UNK:O	23:Ae:283:UNK:HG3	1.95	0.67
46:BA:275:G:O4'	48:BD:260:LYS:NZ	2.28	0.67
73:Bh:60:ARG:NH1	73:Bh:63:LYS:HB2	2.10	0.67
2:AB:114:ILE:HD12	20:Ab:63:ILE:HD12	1.77	0.66
5:AF:53:ALA:HB1	5:AF:54:HIS:HD2	1.59	0.66
21:Ac:48:VAL:HA	21:Ac:52:ILE:HG13	1.75	0.66
66:Ba:200:ARG:HD2	66:Ba:233:LYS:HD3	1.76	0.66
23:Ae:38:UNK:C	23:Ae:41:UNK:HG3	2.25	0.66
46:BA:588:U:OP1	80:Bo:66:ARG:NH2	2.28	0.66
48:BD:114:PRO:HA	48:BD:123:PHE:CZ	2.30	0.66
66:Ba:391:VAL:HG13	66:Ba:399:GLU:HB2	1.75	0.66
67:Bb:259:PRO:HG2	67:Bb:323:TRP:HA	1.77	0.66
17:AY:52:Y5P:H4A	17:AY:53:Y5P:H4	1.78	0.66
32:Ao:174:UNK:HA	32:Ao:177:UNK:HG3	1.76	0.66
32:Ao:485:UNK:O	32:Ao:489:UNK:CG	2.40	0.66
33:Ap:79:ARG:NH1	33:Ap:90:THR:HG22	2.11	0.66
68:Bc:181:VAL:HG22	68:Bc:290:VAL:HG22	1.76	0.66
88:Bz:311:UNK:O	88:Bz:314:UNK:HG3	1.96	0.66
14:AQ:18:ILE:HG12	14:AQ:29:ARG:HB2	1.76	0.66
17:AV:54:Y5P:H4A	17:AV:55:Y5P:H4	1.77	0.66
23:Ae:143:UNK:O	23:Ae:147:UNK:HG2	1.95	0.66
46:BA:575:A:OP1	61:BU:82:LYS:NZ	2.28	0.66
60:BT:114:GLY:HA3	60:BT:182:ARG:HG3	1.78	0.66
72:Bg:14:VAL:HG11	72:Bg:25:GLN:HG3	1.76	0.66
86:Bw:401:ASP:O	86:Bw:402:ASN:ND2	2.28	0.66
1:AA:368:A:O2'	16:AU:42:ARG:NH2	2.29	0.66
92:AA:8139:HOH:O	17:AY:34:P5P:OP2	2.12	0.66
21:Ac:76:LEU:HB2	21:Ac:88:VAL:HB	1.76	0.66
23:Ae:93:UNK:O	23:Ae:96:UNK:HG3	1.94	0.66
23:Ae:354:UNK:CG	23:Ae:357:UNK:CG	2.74	0.66
50:BF:130:GLN:HE22	50:BF:137:ARG:HD2	1.60	0.66
1:AA:86:A:O2'	13:AP:13:ARG:O	2.13	0.66
6:AG:233:ASN:HB3	6:AG:236:LEU:HD12	1.77	0.66
25:Ag:63:UNK:C	25:Ag:64:UNK:HG3	2.25	0.66
32:Ao:336:UNK:HB1	32:Ao:372:UNK:HG1	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:B6:42:THR:HG23	42:B6:55:LEU:HD13	1.76	0.66
46:BA:1290:A:N6	46:BA:1302:G:O2'	2.29	0.66
55:BO:38:VAL:HG21	55:BO:75:LEU:HD11	1.76	0.66
57:BQ:124:VAL:HA	57:BQ:158:ARG:HH21	1.60	0.66
62:BV:180:LYS:HB3	62:BV:181:ARG:NH1	2.11	0.66
74:Bi:90:PRO:HB2	74:Bi:269:TRP:HH2	1.61	0.66
1:AA:747:C:H2'	1:AA:748:A:H5"	1.78	0.66
19:Aa:322:UNK:CG	19:Aa:325:UNK:HG2	2.26	0.66
57:BQ:106:ARG:HB3	57:BQ:106:ARG:NH1	2.11	0.66
66:Ba:340:VAL:HB	66:Ba:359:LEU:HB3	1.77	0.66
1:AA:300:G:N7	92:AA:8061:HOH:O	2.29	0.66
4:AE:365:LYS:HE3	4:AE:366:LYS:HE2	1.76	0.66
7:AI:374:ASP:OD1	7:AI:376:ARG:NH1	2.29	0.66
21:Ac:36:THR:H	21:Ac:69:ASN:ND2	1.88	0.66
23:Ae:170:UNK:CG	28:Aj:78:ARG:HH22	2.09	0.66
27:Ai:17:ARG:NH1	35:Az:697:UNK:HA	2.10	0.66
32:Ao:672:UNK:HA	32:Ao:675:UNK:HG3	1.78	0.66
38:B2:88:THR:HB	38:B2:91:GLN:HG3	1.77	0.66
42:B6:30:PHE:HZ	46:BA:1240:U:C2	2.12	0.66
48:BD:111:ARG:HE	48:BD:152:ILE:HD12	1.61	0.66
56:BP:20:PRO:HD3	83:Bt:99:ARG:HH12	1.61	0.66
58:BR:142:ASN:O	58:BR:148:GLN:NE2	2.28	0.66
59:BS:68:TRP:HB3	59:BS:71:VAL:HG23	1.76	0.66
88:Bz:26:UNK:O	88:Bz:30:UNK:HG3	1.96	0.66
48:BD:263:ARG:HB2	48:BD:263:ARG:NH1	2.06	0.66
73:Bh:259:ARG:HB2	73:Bh:271:PHE:HB2	1.78	0.66
86:Bw:241:LEU:HD13	86:Bw:421:ASN:HD22	1.60	0.66
11:AN:58:ARG:HH12	11:AN:59:LYS:HE2	1.60	0.66
56:BP:141:VAL:HG11	67:Bb:377:TYR:CE1	2.30	0.66
67:Bb:252:CYS:SG	67:Bb:286:ARG:HG3	2.35	0.66
68:Bc:78:MET:HE3	74:Bi:279:THR:HG21	1.78	0.66
6:AG:98:MET:HE1	6:AG:110:LEU:HB2	1.78	0.65
49:BE:236:THR:HA	49:BE:239:ARG:HD2	1.77	0.65
64:BX:14:ASN:HD21	65:BY:211:LYS:H	1.42	0.65
19:Aa:198:ARG:HH11	19:Aa:201:ARG:HE	1.44	0.65
46:BA:186:G:H2'	46:BA:1023:A:N7	2.11	0.65
59:BS:56:LEU:HB3	59:BS:62:ALA:HB2	1.77	0.65
64:BX:18:ARG:NH2	65:BY:206:GLU:OE1	2.29	0.65
74:Bi:147:GLU:HB3	74:Bi:163:LEU:HD11	1.78	0.65
32:Ao:496:UNK:HA	32:Ao:499:UNK:HG3	1.76	0.65
32:Ao:553:UNK:HA	32:Ao:556:UNK:HB1	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:BA:185:U:OP1	46:BA:431:A:O2'	2.14	0.65
46:BA:234:A:H4'	56:BP:34:ARG:HD3	1.77	0.65
64:BX:50:ARG:HH12	64:BX:69:ARG:HA	1.60	0.65
68:Bc:75:VAL:HB	74:Bi:282:ILE:HB	1.78	0.65
23:Ae:135:UNK:O	23:Ae:135:UNK:HG2	1.95	0.65
23:Ae:230:UNK:O	23:Ae:230:UNK:HG2	1.94	0.65
37:B1:91:TYR:CE2	51:BI:79:VAL:HG11	2.31	0.65
46:BA:226:U:O2'	46:BA:229:G:H4'	1.97	0.65
74:Bi:165:THR:HG23	74:Bi:167:ASN:H	1.62	0.65
1:AA:201:A:OP1	22:Ad:64:ARG:NH2	2.30	0.65
17:AY:25:Y5P:C4	17:AY:26:Y5P:H4	2.24	0.65
32:Ao:323:UNK:O	32:Ao:326:UNK:HG3	1.96	0.65
76:Bk:147:ASP:N	76:Bk:147:ASP:OD1	2.28	0.65
14:AQ:55:LEU:HB2	14:AQ:57:GLN:HB2	1.77	0.65
17:AV:26:Y5P:H4A	17:AV:27:Y5P:H4	1.77	0.65
23:Ae:124:UNK:HA	23:Ae:127:UNK:HG3	1.78	0.65
23:Ae:272:UNK:HG2	23:Ae:272:UNK:O	1.97	0.65
25:Ag:284:GLU:OE2	25:Ag:293:ARG:NH1	2.28	0.65
32:Ao:457:UNK:O	32:Ao:460:UNK:HG3	1.96	0.65
67:Bb:108:GLN:HA	67:Bb:111:ARG:HD2	1.76	0.65
88:Bz:412:UNK:O	88:Bz:415:UNK:HG3	1.97	0.65
19:Aa:317:UNK:CG	19:Aa:318:UNK:N	2.59	0.65
23:Ae:91:UNK:O	23:Ae:95:UNK:HG3	1.96	0.65
46:BA:112:A:N6	46:BA:115:U:OP2	2.23	0.65
46:BA:476:A:O2'	62:BV:192:ASN:ND2	2.29	0.65
46:BA:689:A:OP2	92:BA:1929:HOH:O	2.15	0.65
63:BW:123:GLN:HE21	63:BW:135:ARG:HB2	1.60	0.65
23:Ae:29:UNK:O	23:Ae:32:UNK:HG3	1.97	0.65
46:BA:1251:G:O6	56:BP:77:ARG:NH2	2.30	0.65
67:Bb:214:TRP:HB2	67:Bb:240:ILE:HB	1.77	0.65
68:Bc:143:CYS:SG	68:Bc:297:SER:OG	2.52	0.65
85:Bv:114:ARG:NH2	85:Bv:118:GLU:OE2	2.30	0.65
17:AV:34:P5P:H8	17:AV:34:P5P:OP1	1.96	0.65
20:Ab:98:ARG:HB3	20:Ab:125:LEU:HD21	1.77	0.65
23:Ae:54:UNK:HA	23:Ae:57:UNK:HG3	1.78	0.65
23:Ae:369:UNK:O	23:Ae:373:UNK:HG2	1.97	0.65
59:BS:91:GLU:HG2	59:BS:93:LEU:HD21	1.79	0.65
63:BW:76:ARG:HA	63:BW:171:HIS:HD2	1.60	0.65
23:Ae:81:UNK:O	23:Ae:82:UNK:CG	2.44	0.65
46:BA:690:A:H2'	46:BA:691:U:H5'	1.78	0.65
74:Bi:245:TYR:HD1	74:Bi:265:ILE:HB	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:Bj:116:LEU:N	75:Bj:119:ASP:OD2	2.30	0.65
80:Bo:65:ARG:HB2	80:Bo:65:ARG:HH11	1.62	0.65
86:Bw:278:ILE:HD11	86:Bw:333:GLN:HG2	1.79	0.65
1:AA:318:C:H3'	15:AR:106:LYS:HZ3	1.61	0.64
8:AJ:91:TYR:OH	8:AJ:160:ILE:O	2.14	0.64
25:Ag:66:UNK:O	25:Ag:66:UNK:HG2	1.97	0.64
25:Ag:161:VAL:HG22	25:Ag:289:ILE:HD11	1.79	0.64
25:Ag:243:LEU:HG	25:Ag:295:MET:HE3	1.79	0.64
32:Ao:190:UNK:HG1	32:Ao:223:UNK:HB2	1.79	0.64
55:BO:93:GLY:O	55:BO:95:ARG:NH1	2.26	0.64
59:BS:130:ARG:NH1	67:Bb:129:ARG:HH11	1.94	0.64
61:BU:146:VAL:HG11	71:Bf:56:ARG:HG2	1.80	0.64
4:AE:371:VAL:HG22	4:AE:383:VAL:HG22	1.79	0.64
17:AV:9:Y5P:O2'	17:AV:10:Y5P:C5	2.45	0.64
19:Aa:323:UNK:O	19:Aa:327:UNK:HG3	1.97	0.64
23:Ae:222:UNK:HG1	23:Ae:299:UNK:HG2	1.79	0.64
32:Ao:674:UNK:O	32:Ao:677:UNK:HG3	1.97	0.64
46:BA:657:U:O2'	58:BR:82:GLU:OE2	2.14	0.64
46:BA:879:C:H4'	46:BA:880:A:H5'	1.78	0.64
68:Bc:153:ARG:O	71:Bf:90:UNK:CG	2.45	0.64
73:Bh:259:ARG:HH11	73:Bh:259:ARG:CG	1.99	0.64
4:AE:302:HIS:HB2	4:AE:337:SER:HB2	1.79	0.64
23:Ae:230:UNK:O	23:Ae:231:UNK:CG	2.39	0.64
32:Ao:82:SER:O	32:Ao:446:UNK:CG	2.45	0.64
32:Ao:510:UNK:HG2	32:Ao:511:UNK:N	2.12	0.64
68:Bc:105:VAL:HG22	68:Bc:122:ILE:HG12	1.79	0.64
71:Bf:88:UNK:C	71:Bf:91:UNK:HG3	2.27	0.64
73:Bh:59:ARG:HB2	73:Bh:62:GLU:HG3	1.79	0.64
25:Ag:154:ILE:HD13	25:Ag:261:VAL:HG22	1.78	0.64
32:Ao:340:UNK:O	32:Ao:343:UNK:HG3	1.96	0.64
33:Ap:74:TRP:HB3	33:Ap:106:PRO:HG3	1.78	0.64
40:B4:58:VAL:HB	40:B4:77:THR:HG23	1.79	0.64
60:BT:60:UNK:HG2	60:BT:60:UNK:O	1.98	0.64
83:Bt:9:ARG:HH11	83:Bt:9:ARG:HG3	1.61	0.64
8:AJ:64:THR:CG2	32:Ao:64:THR:O	2.42	0.64
17:AV:9:Y5P:O2'	17:AV:10:Y5P:H5	1.97	0.64
17:AY:54:Y5P:H4A	17:AY:55:Y5P:H4A	1.78	0.64
23:Ae:84:UNK:HG2	23:Ae:86:UNK:HG3	1.78	0.64
38:B2:93:ARG:HH12	70:Be:82:THR:C	2.04	0.64
46:BA:40:C:H42	66:Ba:89:ARG:HH21	1.42	0.64
46:BA:455:G:N7	92:BA:1861:HOH:O	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:BA:747:C:O2'	46:BA:748:A:H5"	1.97	0.64
2:AB:140:ILE:HB	2:AB:189:PRO:HA	1.80	0.64
17:AV:49:Y5P:H4A	17:AV:50:Y5P:H4	1.80	0.64
22:Ad:189:TRP:HE1	22:Ad:197:VAL:HB	1.63	0.64
28:Aj:121:LYS:HE3	28:Aj:123:LYS:HZ1	1.61	0.64
29:Ak:165:ILE:H	32:Ao:134:GLU:HB2	1.62	0.64
66:Ba:353:GLN:NE2	66:Ba:379:ASP:OD1	2.30	0.64
73:Bh:32:LYS:NZ	79:Bn:42:LYS:NZ	2.46	0.64
73:Bh:88:LEU:HD21	73:Bh:198:VAL:HG13	1.78	0.64
73:Bh:148:LEU:HD22	73:Bh:305:PHE:HB3	1.80	0.64
25:Ag:312:THR:OG1	92:Ag:502:HOH:O	2.15	0.64
32:Ao:225:UNK:HG1	32:Ao:263:UNK:HB1	1.79	0.64
32:Ao:318:UNK:HA	32:Ao:321:UNK:HG3	1.79	0.64
56:BP:229:PHE:O	56:BP:233:ARG:HB3	1.97	0.64
77:Bl:111:ARG:HB3	77:Bl:111:ARG:HH11	1.63	0.64
81:Bp:16:VAL:HG13	81:Bp:66:VAL:HG22	1.80	0.64
17:AV:66:Y5P:H4A	17:AV:67:Y5P:C4	2.27	0.64
46:BA:58:C:H2'	46:BA:59:A:H5"	1.79	0.64
49:BE:90:TRP:HA	49:BE:316:PHE:HE2	1.62	0.64
57:BQ:50:LEU:H	57:BQ:110:ASN:HD21	1.45	0.64
73:Bh:105:ARG:NH1	73:Bh:116:LEU:HD23	2.11	0.64
8:AJ:123:SER:O	11:AN:108:ARG:NH2	2.31	0.64
23:Ae:48:UNK:HB2	23:Ae:53:UNK:CG	2.28	0.64
29:Ak:118:PRO:O	29:Ak:122:LYS:HG2	1.98	0.64
30:Am:31:ASN:HB3	30:Am:109:HIS:CE1	2.33	0.64
31:An:193:LYS:HD2	31:An:196:LEU:HB2	1.79	0.64
32:Ao:598:UNK:HB2	32:Ao:655:UNK:HB2	1.80	0.64
41:B5:90:ASN:O	41:B5:94:ARG:HG2	1.98	0.64
42:B6:44:LEU:HB3	42:B6:53:LYS:HE3	1.79	0.64
1:AA:571:A:H2'	1:AA:572:A:C8	2.32	0.64
21:Ac:47:PHE:HA	21:Ac:51:ASN:HD22	1.63	0.64
37:B1:116:SER:HB3	37:B1:119:LEU:HB2	1.80	0.64
42:B6:34:ARG:HG3	42:B6:36:ARG:HG2	1.80	0.64
48:BD:73:THR:HG22	48:BD:75:MET:H	1.63	0.64
50:BF:240:PHE:O	50:BF:241:ASN:ND2	2.31	0.64
81:Bp:73:ARG:HB3	87:Bx:46:THR:HG22	1.80	0.64
23:Ae:163:UNK:CG	23:Ae:206:UNK:HB2	2.27	0.63
46:BA:658:C:N4	86:Bw:54:LYS:HB3	2.13	0.63
1:AA:59:C:C2	28:Aj:136:TYR:HB2	2.33	0.63
1:AA:257:U:H4'	1:AA:258:C:H5'	1.79	0.63
28:Aj:96:ARG:O	28:Aj:117:ILE:N	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:BA:15:A:H2'	46:BA:16:A:H8	1.64	0.63
46:BA:215:C:OP2	77:Bl:111:ARG:NH2	2.31	0.63
46:BA:562:A:OP1	83:Bt:9:ARG:NH2	2.29	0.63
48:BD:263:ARG:HH11	48:BD:263:ARG:CB	2.05	0.63
49:BE:96:ARG:CB	49:BE:96:ARG:HH11	2.11	0.63
57:BQ:131:ILE:HB	57:BQ:149:HIS:HB2	1.79	0.63
66:Ba:194:LYS:HG2	66:Ba:195:HIS:HD2	1.62	0.63
67:Bb:251:THR:HG23	67:Bb:285:THR:HA	1.80	0.63
88:Bz:19:UNK:C	88:Bz:22:UNK:HG3	2.28	0.63
1:AA:790:A:OP1	7:AI:389:ARG:NH1	2.29	0.63
19:Aa:323:UNK:CG	19:Aa:324:UNK:N	2.61	0.63
32:Ao:222:UNK:HA	32:Ao:225:UNK:HG3	1.80	0.63
32:Ao:227:UNK:HA	32:Ao:230:UNK:HG3	1.81	0.63
46:BA:303:U:H2'	46:BA:304:G:O4'	1.99	0.63
62:BV:198:ARG:NH2	72:Bg:17:ASN:O	2.32	0.63
65:BY:129:LYS:HD3	65:BY:149:ARG:HH21	1.63	0.63
66:Ba:147:ILE:HG22	66:Ba:148:GLU:H	1.62	0.63
68:Bc:278:SER:O	68:Bc:317:ARG:NH1	2.31	0.63
19:Aa:262:ARG:HH22	19:Aa:287:GLN:HG3	1.63	0.63
23:Ae:76:UNK:HA	23:Ae:79:UNK:HG3	1.80	0.63
29:Ak:73:PRO:HB3	32:Ao:78:VAL:HG11	1.81	0.63
32:Ao:415:UNK:O	32:Ao:418:UNK:HG3	1.98	0.63
74:Bi:105:LEU:HD22	74:Bi:193:GLN:HE21	1.63	0.63
86:Bw:118:LEU:HG	86:Bw:119:PRO:HD2	1.78	0.63
17:AY:31:Y5P:H4A	17:AY:32:Y5P:H4	1.81	0.63
24:Af:105:ILE:HG12	24:Af:115:ILE:HG12	1.81	0.63
46:BA:694:A:H3'	46:BA:695:C:H5"	1.80	0.63
72:Bg:44:ARG:NH1	83:Bt:99:ARG:O	2.31	0.63
73:Bh:32:LYS:HZ3	79:Bn:42:LYS:HZ3	1.46	0.63
87:Bx:72:ILE:HG13	87:Bx:111:GLU:HG2	1.80	0.63
12:AO:74:LEU:HG	12:AO:94:LEU:O	1.98	0.63
12:AO:172:ARG:HH12	14:AQ:88:VAL:HG21	1.63	0.63
17:AY:24:Y5P:H4A	17:AY:25:Y5P:H4	1.81	0.63
19:Aa:141:LEU:HB2	19:Aa:180:LEU:HD23	1.81	0.63
23:Ae:238:UNK:HG2	23:Ae:238:UNK:O	1.98	0.63
23:Ae:359:UNK:C	23:Ae:362:UNK:HG3	2.28	0.63
32:Ao:361:UNK:HA	32:Ao:364:UNK:HG3	1.80	0.63
40:B4:38:ARG:NH1	69:Bd:132:GLU:OE1	2.32	0.63
46:BA:32:C:O2'	46:BA:36:A:N6	2.31	0.63
46:BA:65:C:N4	92:BA:1924:HOH:O	2.15	0.63
46:BA:1431:U:H4'	46:BA:1432:U:H5'	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:BY:64:ILE:HD11	65:BY:88:VAL:HG21	1.81	0.63
76:Bk:171:LEU:HA	76:Bk:174:ILE:HD12	1.81	0.63
88:Bz:405:UNK:O	88:Bz:408:UNK:CG	2.46	0.63
1:AA:492:U:OP1	31:An:139:ASN:ND2	2.32	0.63
3:AC:112:ARG:HB2	3:AC:112:ARG:HH11	1.62	0.63
42:B6:45:HIS:CD2	42:B6:46:TYR:H	2.16	0.63
45:B9:74:ARG:NH1	46:BA:543:U:O2'	2.32	0.63
46:BA:658:C:H41	86:Bw:54:LYS:HB3	1.64	0.63
48:BD:172:ARG:HB2	48:BD:173:MET:SD	2.39	0.63
50:BF:279:ARG:NH1	50:BF:286:PHE:CE2	2.67	0.63
56:BP:94:GLN:NE2	56:BP:128:THR:O	2.31	0.63
68:Bc:62:ILE:HD11	68:Bc:118:LYS:C	2.24	0.63
74:Bi:170:PRO:O	74:Bi:174:TRP:HB2	1.98	0.63
17:AY:37:Y5P:HB	17:AY:38:Y5P:H6	1.81	0.63
17:AY:44:Y5P:H4A	17:AY:45:Y5P:H4	1.81	0.63
19:Aa:348:UNK:HA	19:Aa:351:UNK:HG3	1.81	0.63
23:Ae:175:UNK:HG1	23:Ae:368:UNK:HG3	1.80	0.63
52:BJ:85:GLU:OE2	82:Bq:115:ARG:NH2	2.32	0.63
67:Bb:217:LEU:HD13	67:Bb:236:LEU:HD13	1.80	0.63
86:Bw:278:ILE:HG22	86:Bw:280:SER:H	1.64	0.63
13:AP:54:TYR:HD1	13:AP:66:VAL:HG22	1.64	0.63
19:Aa:314:UNK:HA	19:Aa:317:UNK:HG3	1.81	0.63
25:Ag:294:LYS:HG2	25:Ag:297:LYS:NZ	2.14	0.63
28:Aj:64:LEU:HD23	28:Aj:134:VAL:HG13	1.80	0.63
46:BA:775:A:OP1	86:Bw:62:ARG:HD2	1.99	0.63
46:BA:1449:U:O2'	55:BO:63:LYS:NZ	2.22	0.63
46:BA:1528:C:H1'	87:Bx:133:PRO:HD2	1.80	0.63
49:BE:95:SER:HB2	49:BE:303:LYS:NZ	2.13	0.63
55:BO:55:PRO:HB3	55:BO:77:ILE:HG23	1.81	0.63
62:BV:98:ARG:HH11	62:BV:113:THR:HG21	1.64	0.63
19:Aa:94:LEU:HB2	33:Ap:166:HIS:HB2	1.81	0.62
25:Ag:120:ALA:HB3	25:Ag:298:ASN:HA	1.80	0.62
32:Ao:303:UNK:HG1	32:Ao:340:UNK:HG2	1.81	0.62
32:Ao:532:UNK:O	32:Ao:535:UNK:HG3	1.99	0.62
32:Ao:538:UNK:O	32:Ao:550:UNK:CG	2.44	0.62
46:BA:546:A:H5"	82:Bq:126:ILE:HD11	1.81	0.62
46:BA:1349:U:H2'	46:BA:1351:C:H5"	1.80	0.62
63:BW:88:LEU:HD21	63:BW:109:LYS:HG3	1.80	0.62
74:Bi:186:VAL:HG13	74:Bi:219:ARG:HB3	1.81	0.62
7:AI:383:PRO:HB2	8:AJ:131:ARG:HB2	1.81	0.62
32:Ao:360:UNK:C	32:Ao:363:UNK:HG3	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:BA:1440:U:H5”	49:BE:253:PRO:HA	1.81	0.62
48:BD:114:PRO:HA	48:BD:123:PHE:CE1	2.34	0.62
51:BI:59:TRP:HE1	51:BI:81:LYS:HB3	1.64	0.62
54:BN:142:VAL:HG12	54:BN:143:GLU:HB3	1.80	0.62
68:Bc:45:PHE:HD2	68:Bc:253:ARG:HH11	1.46	0.62
1:AA:552:A:H2’	1:AA:553:G:C8	2.34	0.62
4:AE:126:LEU:HD13	27:Ai:77:ASP:HB3	1.81	0.62
23:Ae:129:UNK:O	23:Ae:133:UNK:HG2	1.99	0.62
32:Ao:374:UNK:HA	32:Ao:377:UNK:HG3	1.81	0.62
46:BA:924:U:O2’	46:BA:925:A:H8	1.82	0.62
1:AA:513:A:N3	1:AA:857:C:O2’	2.31	0.62
54:BN:174:GLU:HA	87:Bx:56:THR:HG21	1.81	0.62
67:Bb:213:LEU:HB3	67:Bb:275:GLN:HG3	1.81	0.62
85:Bv:142:ARG:HA	85:Bv:145:UNK:HG3	1.80	0.62
1:AA:591:A:H61	1:AA:704:U:H3	1.45	0.62
23:Ae:243:UNK:O	23:Ae:244:UNK:CG	2.48	0.62
40:B4:52:LEU:HG	40:B4:68:ARG:HB3	1.81	0.62
60:BT:59:UNK:HG2	60:BT:59:UNK:O	1.99	0.62
68:Bc:35:THR:HA	68:Bc:38:ILE:HD12	1.82	0.62
82:Bq:103:PRO:HG2	82:Bq:105:LYS:HE3	1.80	0.62
1:AA:164:C:H4’	28:Aj:18:VAL:HG11	1.82	0.62
1:AA:654:A:H2’	1:AA:655:G:H5’	1.81	0.62
3:AC:148:LYS:NZ	32:Ao:128:PHE:O	2.31	0.62
14:AQ:57:GLN:HE21	14:AQ:87:LYS:NZ	1.97	0.62
25:Ag:56:UNK:HB2	25:Ag:146:LYS:NZ	2.14	0.62
28:Aj:145:HIS:CD2	28:Aj:146:GLU:HG2	2.35	0.62
30:Am:49:MET:O	30:Am:53:MET:HG2	1.99	0.62
32:Ao:204:UNK:HA	32:Ao:207:UNK:CG	2.29	0.62
32:Ao:300:UNK:HA	32:Ao:303:UNK:HG3	1.80	0.62
32:Ao:580:UNK:HA	32:Ao:583:UNK:HG3	1.80	0.62
38:B2:128:MET:HE3	38:B2:131:PRO:HA	1.81	0.62
46:BA:48:U:C1’	51:BI:78:ARG:HH12	2.12	0.62
56:BP:55:GLY:O	56:BP:59:ARG:NH1	2.32	0.62
69:Bd:164:ARG:HH11	76:Bk:88:TYR:HB3	1.62	0.62
81:Bp:11:ARG:HA	81:Bp:46:ASN:HB3	1.81	0.62
19:Aa:182:LYS:NZ	33:Ap:183:ALA:HA	2.14	0.62
19:Aa:351:UNK:HA	19:Aa:354:UNK:HG3	1.81	0.62
46:BA:1002:A:N6	92:BA:1815:HOH:O	2.33	0.62
54:BN:154:ARG:HB2	54:BN:154:ARG:HH11	1.65	0.62
57:BQ:124:VAL:HG22	57:BQ:158:ARG:HE	1.64	0.62
64:BX:24:PHE:HD2	64:BX:45:PRO:HG2	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:Ba:212:THR:HG21	66:Ba:273:VAL:HG22	1.81	0.62
7:AI:266:UNK:HG1	7:AI:268:MET:HE2	1.82	0.62
11:AN:52:LEU:O	11:AN:56:SER:OG	2.17	0.62
21:Ac:51:ASN:ND2	21:Ac:95:ASN:OD1	2.31	0.62
23:Ae:230:UNK:C	23:Ae:231:UNK:HG3	2.27	0.62
24:Af:153:ARG:NH2	24:Af:158:THR:O	2.29	0.62
32:Ao:476:UNK:HB1	32:Ao:506:UNK:HG1	1.80	0.62
37:B1:92:VAL:HG23	37:B1:98:SER:HB3	1.81	0.62
46:BA:1508:A:O3'	87:Bx:160:LYS:NZ	2.33	0.62
57:BQ:67:LYS:HD2	57:BQ:69:LEU:HD21	1.82	0.62
64:BX:141:ARG:NH1	74:Bi:276:ILE:HD11	2.15	0.62
69:Bd:143:GLN:NE2	75:Bj:210:CYS:O	2.32	0.62
73:Bh:123:GLN:O	73:Bh:126:SER:OG	2.17	0.62
4:AE:224:GLU:HB2	4:AE:342:MET:HG2	1.81	0.62
19:Aa:340:UNK:HA	19:Aa:343:UNK:HG3	1.80	0.62
38:B2:80:LYS:NZ	74:Bi:71:ARG:HH21	1.97	0.62
60:BT:68:UNK:HG2	60:BT:68:UNK:O	2.00	0.62
88:Bz:307:UNK:O	88:Bz:310:UNK:HG3	2.00	0.62
3:AC:53:TYR:HB2	29:Ak:99:MET:HE1	1.82	0.62
3:AC:62:ILE:HG12	3:AC:66:LYS:HD3	1.82	0.62
4:AE:304:LYS:NZ	4:AE:410:ASP:OD1	2.25	0.62
19:Aa:261:LEU:HD22	19:Aa:266:HIS:HB2	1.82	0.62
32:Ao:244:UNK:O	32:Ao:247:UNK:HG3	1.98	0.62
32:Ao:484:UNK:O	32:Ao:487:UNK:HG3	1.99	0.62
42:B6:17:LEU:HD22	46:BA:1242:U:H4'	1.82	0.62
14:AQ:14:VAL:H	21:Ac:63:GLN:HE22	1.48	0.61
46:BA:87:A:OP1	79:Bn:118:TYR:OH	2.14	0.61
46:BA:479:G:H4'	61:BU:98:ASN:HD21	1.64	0.61
85:Bv:48:PRO:HB2	85:Bv:50:TRP:CD1	2.35	0.61
2:AB:133:HIS:HB3	20:Ab:34:ILE:HD13	1.81	0.61
3:AC:88:GLU:HG3	3:AC:147:TYR:CZ	2.36	0.61
23:Ae:81:UNK:C	23:Ae:82:UNK:HG3	2.31	0.61
32:Ao:459:UNK:O	32:Ao:462:UNK:HG3	2.01	0.61
46:BA:185:U:O4'	46:BA:432:G:O2'	2.15	0.61
46:BA:387:A:OP2	83:Bt:81:ARG:NH1	2.33	0.61
46:BA:1258:U:H2'	46:BA:1259:U:C6	2.35	0.61
63:BW:133:GLU:HG2	74:Bi:278:LYS:HB2	1.82	0.61
1:AA:671:U:H2'	1:AA:672:A:H8	1.64	0.61
23:Ae:268:UNK:HG3	33:Ap:214:SER:HG	1.64	0.61
32:Ao:499:UNK:O	32:Ao:503:UNK:HG3	2.00	0.61
46:BA:579:A:H5"	80:Bo:23:ALA:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:BJ:100:GLN:HB2	52:BJ:177:LEU:HD11	1.83	0.61
60:BT:276:SER:HA	60:BT:279:GLU:HG3	1.82	0.61
67:Bb:175:VAL:HB	67:Bb:187:VAL:HB	1.82	0.61
8:AJ:78:VAL:HG22	8:AJ:172:VAL:HG22	1.82	0.61
12:AO:144:MET:HE2	12:AO:144:MET:HA	1.81	0.61
19:Aa:207:VAL:O	19:Aa:213:ASN:ND2	2.33	0.61
23:Ae:108:UNK:O	23:Ae:112:UNK:HG3	2.00	0.61
28:Aj:27:ARG:NH1	28:Aj:33:ARG:NH1	2.46	0.61
37:B1:238:LEU:HD13	70:Be:102:PHE:HD2	1.65	0.61
39:B3:74:SER:HB2	46:BA:471:U:H5"	1.82	0.61
69:Bd:169:PHE:HB2	69:Bd:170:PRO:HD3	1.82	0.61
88:Bz:309:UNK:O	88:Bz:313:UNK:HG3	2.01	0.61
4:AE:160:ARG:NH1	4:AE:168:VAL:HG21	2.14	0.61
23:Ae:181:UNK:HG1	23:Ae:210:UNK:HG3	1.76	0.61
23:Ae:220:UNK:O	23:Ae:224:UNK:HG3	2.01	0.61
32:Ao:161:UNK:HB2	32:Ao:170:UNK:HB2	1.82	0.61
56:BP:54:LYS:O	56:BP:58:GLN:HB2	2.00	0.61
62:BV:117:LEU:HD13	62:BV:198:ARG:NH1	2.16	0.61
63:BW:67:ARG:NE	74:Bi:228:PHE:O	2.32	0.61
68:Bc:246:GLU:HB2	68:Bc:248:ILE:HG13	1.83	0.61
17:AY:55:Y5P:C5	17:AY:58:Y5P:C5	2.79	0.61
23:Ae:257:UNK:HG1	23:Ae:288:UNK:HG1	1.80	0.61
48:BD:74:VAL:HG13	48:BD:151:TRP:HE1	1.65	0.61
62:BV:134:LEU:HB2	62:BV:160:VAL:HG13	1.82	0.61
66:Ba:343:GLN:HG2	66:Ba:356:VAL:HG22	1.83	0.61
67:Bb:178:ALA:HB2	84:Bu:194:SER:HB2	1.81	0.61
1:AA:131:U:O2'	14:AQ:23:GLN:NE2	2.33	0.61
23:Ae:124:UNK:C	23:Ae:127:UNK:HG3	2.30	0.61
27:Ai:17:ARG:NH2	29:Ak:234:GLU:OE2	2.33	0.61
28:Aj:178:ARG:NH2	28:Aj:187:GLU:O	2.33	0.61
29:Ak:264:ILE:HD11	29:Ak:294:TYR:CG	2.35	0.61
57:BQ:36:VAL:HG23	82:Bq:128:ARG:HD2	1.82	0.61
83:Bt:90:GLU:N	83:Bt:90:GLU:OE1	2.34	0.61
17:AY:66:Y5P:H4A	17:AY:67:Y5P:H4	1.82	0.61
23:Ae:68:UNK:HG2	23:Ae:71:UNK:CG	2.30	0.61
23:Ae:219:UNK:HA	23:Ae:222:UNK:HG3	1.81	0.61
36:B0:57:GLU:OE1	36:B0:99:TYR:N	2.32	0.61
46:BA:163:A:H2'	61:BU:35:LYS:NZ	2.15	0.61
46:BA:406:A:OP2	76:Bk:49:ARG:NH1	2.34	0.61
46:BA:446:A:H5'	46:BA:447:G:OP2	2.00	0.61
50:BF:71:GLY:H	50:BF:74:GLN:NE2	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:BN:117:HIS:O	54:BN:121:MET:HG2	2.01	0.61
67:Bb:195:PRO:HA	67:Bb:198:ALA:HB3	1.82	0.61
69:Bd:164:ARG:HB3	76:Bk:86:TYR:CE1	2.35	0.61
85:Bv:148:UNK:HA	85:Bv:151:UNK:HG3	1.81	0.61
86:Bw:77:ASP:N	86:Bw:77:ASP:OD1	2.29	0.61
88:Bz:421:UNK:HA	88:Bz:424:UNK:CG	2.30	0.61
2:AB:141:ILE:HG12	2:AB:191:LEU:HB3	1.83	0.61
14:AQ:96:THR:HG23	22:Ad:120:ARG:HH11	1.65	0.61
32:Ao:507:UNK:HG1	32:Ao:541:UNK:HB1	1.83	0.61
32:Ao:517:UNK:O	32:Ao:520:UNK:HG3	2.01	0.61
46:BA:192:U:H2'	46:BA:193:G:C8	2.36	0.61
50:BF:230:VAL:O	50:BF:234:THR:OG1	2.17	0.61
56:BP:195:LEU:HD21	56:BP:277:MET:HE2	1.83	0.61
69:Bd:171:PHE:HB3	76:Bk:186:VAL:HB	1.83	0.61
88:Bz:400:UNK:O	88:Bz:403:UNK:HG3	2.00	0.61
1:AA:43:U:H2'	1:AA:44:U:O4'	2.00	0.61
9:AK:166:GLY:HA2	9:AK:169:MET:HE2	1.83	0.61
17:AY:9:Y5P:H4A	17:AY:22:Y5P:C5	2.31	0.61
23:Ae:48:UNK:HG1	23:Ae:74:UNK:O	2.01	0.61
25:Ag:129:LYS:HE3	25:Ag:312:THR:HG22	1.81	0.61
25:Ag:164:CYS:H	25:Ag:273:LEU:HD21	1.64	0.61
27:Ai:17:ARG:HH21	35:Az:698:UNK:HG3	1.63	0.61
32:Ao:192:UNK:O	32:Ao:195:UNK:HG3	2.00	0.61
52:BJ:40:MET:HE1	52:BJ:48:MET:HE3	1.82	0.61
67:Bb:262:GLY:HA3	67:Bb:342:PHE:HB2	1.83	0.61
75:Bj:46:ARG:HB3	75:Bj:229:ALA:HB2	1.83	0.61
88:Bz:402:UNK:O	88:Bz:406:UNK:HB1	2.01	0.61
1:AA:356:A:H2'	1:AA:357:G:H8	1.66	0.60
1:AA:573:A:C8	1:AA:622:U:H4'	2.36	0.60
24:Af:104:GLN:HG3	24:Af:140:ARG:HG2	1.83	0.60
39:B3:46:PHE:O	83:Bt:50:SER:OG	2.14	0.60
46:BA:718:C:H5'	48:BD:75:MET:HG2	1.83	0.60
46:BA:1255:A:H8	46:BA:1255:A:H3'	1.66	0.60
66:Ba:136:VAL:HG22	66:Ba:420:HIS:HD2	1.66	0.60
72:Bg:73:PRO:HB2	72:Bg:89:ILE:HG13	1.82	0.60
1:AA:356:A:H2'	1:AA:357:G:C8	2.36	0.60
7:AI:150:LEU:O	7:AI:153:THR:OG1	2.17	0.60
23:Ae:399:UNK:HA	23:Ae:402:UNK:HG3	1.82	0.60
39:B3:77:ARG:NH1	46:BA:456:A:H4'	2.15	0.60
44:B8:135:LYS:HD3	46:BA:1229:U:H5'	1.83	0.60
46:BA:276:A:C2'	46:BA:277:A:H5"	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:BA:716:A:H5'	46:BA:717:C:OP2	2.01	0.60
49:BE:175:LYS:HD2	49:BE:296:LEU:HB3	1.82	0.60
60:BT:96:ARG:NH1	60:BT:285:GLU:OE1	2.34	0.60
65:BY:109:ILE:HD13	74:Bi:76:ILE:HG21	1.84	0.60
66:Ba:240:ALA:HB3	66:Ba:358:GLN:HE22	1.66	0.60
74:Bi:100:LEU:HD13	74:Bi:103:GLU:HG3	1.83	0.60
83:Bt:12:ILE:HD13	83:Bt:23:ARG:HB2	1.83	0.60
1:AA:124:A:H1'	1:AA:125:U:C5	2.37	0.60
7:AI:265:UNK:HG2	7:AI:266:UNK:N	2.16	0.60
8:AJ:84:ASP:OD1	8:AJ:84:ASP:N	2.29	0.60
19:Aa:343:UNK:O	19:Aa:346:UNK:CG	2.41	0.60
23:Ae:90:UNK:HG2	23:Ae:91:UNK:N	2.15	0.60
23:Ae:287:UNK:HA	23:Ae:290:UNK:HG3	1.83	0.60
31:An:146:LEU:HD12	31:An:149:ARG:HH12	1.67	0.60
38:B2:232:LYS:NZ	46:BA:10:A:OP1	2.35	0.60
41:B5:140:GLN:HE22	41:B5:176:GLU:C	2.08	0.60
44:B8:101:LYS:HE3	46:BA:75:A:H2	1.65	0.60
46:BA:187:C:H3'	62:BV:181:ARG:NH2	2.15	0.60
58:BR:106:ARG:HE	58:BR:127:LYS:HE2	1.66	0.60
81:Bp:18:VAL:HG22	81:Bp:64:VAL:HG13	1.82	0.60
17:AV:30:Y5P:H2'	17:AV:31:Y5P:H6	1.82	0.60
23:Ae:265:UNK:O	23:Ae:265:UNK:HG3	2.01	0.60
23:Ae:367:UNK:O	23:Ae:370:UNK:HG3	2.02	0.60
32:Ao:605:UNK:HG1	32:Ao:651:UNK:CG	2.31	0.60
34:As:2366:UNK:O	34:As:2370:UNK:HG3	2.00	0.60
46:BA:1334:A:H2'	46:BA:1335:G:C8	2.35	0.60
51:BI:91:LYS:NZ	51:BI:116:LYS:HB2	2.16	0.60
86:Bw:105:TRP:CD1	86:Bw:265:LEU:HD13	2.37	0.60
1:AA:604:U:H1'	27:Ai:95:ARG:HD3	1.83	0.60
16:AU:15:GLN:HG2	16:AU:16:GLU:HG3	1.82	0.60
19:Aa:346:UNK:O	19:Aa:349:UNK:HG3	2.02	0.60
32:Ao:459:UNK:HA	32:Ao:462:UNK:HG3	1.82	0.60
32:Ao:656:UNK:O	32:Ao:660:UNK:CG	2.46	0.60
36:B0:56:MET:H	36:B0:59:HIS:HD2	1.48	0.60
49:BE:76:LYS:NZ	49:BE:168:LEU:HD12	2.16	0.60
56:BP:276:ASN:ND2	56:BP:279:ASP:OD2	2.34	0.60
4:AE:284:ARG:HH11	4:AE:328:GLY:C	2.09	0.60
7:AI:311:ARG:NH1	25:Ag:382:LEU:O	2.34	0.60
10:AL:33:LEU:HD22	14:AQ:39:LEU:HD23	1.82	0.60
23:Ae:390:UNK:HA	23:Ae:393:UNK:HG3	1.83	0.60
25:Ag:173:ASN:O	25:Ag:176:ARG:NH1	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:BA:1253:A:H2'	46:BA:1254:C:C6	2.37	0.60
87:Bx:71:PRO:HD2	87:Bx:107:LEU:HD23	1.83	0.60
23:Ae:243:UNK:C	23:Ae:244:UNK:HG3	2.32	0.60
44:B8:108:LYS:NZ	46:BA:78:A:OP2	2.30	0.60
46:BA:797:A:H61	46:BA:989:C:H42	1.50	0.60
61:BU:11:ARG:NH1	61:BU:13:ARG:HD2	2.16	0.60
65:BY:105:ARG:H	65:BY:105:ARG:HD3	1.67	0.60
87:Bx:35:PHE:CE2	87:Bx:57:PRO:HD2	2.37	0.60
1:AA:223:U:O2'	1:AA:224:U:OP1	2.17	0.60
8:AJ:73:TYR:HE2	8:AJ:150:GLY:HA2	1.66	0.60
15:AR:83:GLN:NE2	15:AR:134:PRO:HG2	2.17	0.60
28:Aj:36:LEU:HD13	28:Aj:43:ARG:HE	1.66	0.60
32:Ao:426:UNK:HA	32:Ao:429:UNK:HG3	1.82	0.60
38:B2:66:LEU:N	38:B2:68:GLU:OE1	2.35	0.60
61:BU:92:LYS:HZ3	80:Bo:27:TRP:CD1	2.19	0.60
68:Bc:206:LEU:HD12	68:Bc:209:LYS:HE3	1.83	0.60
75:Bj:74:LEU:HA	75:Bj:77:ILE:HG22	1.83	0.60
80:Bo:65:ARG:HB2	80:Bo:65:ARG:NH1	2.17	0.60
87:Bx:173:ARG:HB3	87:Bx:195:TYR:HB3	1.83	0.60
1:AA:17:G:H2'	1:AA:18:G:C8	2.37	0.60
23:Ae:365:UNK:O	23:Ae:365:UNK:HG2	2.01	0.60
32:Ao:190:UNK:HG2	32:Ao:227:UNK:HB1	1.84	0.60
45:B9:100:MET:HE3	46:BA:560:A:H5"	1.84	0.60
56:BP:11:ARG:HG2	56:BP:11:ARG:NH1	2.15	0.60
75:Bj:158:ILE:HG21	75:Bj:260:LEU:HD13	1.84	0.60
88:Bz:106:UNK:O	88:Bz:106:UNK:CG	2.46	0.60
1:AA:645:A:H5'	1:AA:646:C:C5	2.37	0.60
17:AV:43:Y5P:H4A	17:AV:44:Y5P:H4	1.82	0.60
17:AY:9:Y5P:C4	17:AY:22:Y5P:H5	2.31	0.60
23:Ae:359:UNK:O	23:Ae:362:UNK:HG3	2.02	0.60
33:Ap:210:GLU:OE2	33:Ap:217:ARG:NH2	2.33	0.60
47:BB:61:Y5P:H4A	47:BB:62:Y5P:H4	1.84	0.60
63:BW:130:HIS:CE1	74:Bi:227:ARG:HH11	2.20	0.60
68:Bc:172:ILE:O	68:Bc:315:ARG:NH1	2.33	0.60
68:Bc:187:ASP:HA	68:Bc:291:ARG:NH2	2.17	0.60
75:Bj:235:LYS:HZ2	76:Bk:172:GLU:HG2	1.65	0.60
5:AF:53:ALA:HB1	5:AF:54:HIS:CD2	2.37	0.59
9:AK:65:TYR:O	9:AK:67:PRO:HD3	2.02	0.59
19:Aa:314:UNK:C	19:Aa:317:UNK:HG3	2.32	0.59
19:Aa:331:UNK:HG2	19:Aa:341:UNK:HG1	1.79	0.59
37:B1:163:ARG:NH1	66:Ba:55:LEU:HD11	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:BY:131:THR:HG23	65:BY:149:ARG:HD2	1.83	0.59
1:AA:389:A:O2'	12:AO:143:HIS:ND1	2.30	0.59
11:AN:58:ARG:HB3	11:AN:58:ARG:NH1	2.16	0.59
17:AY:55:Y5P:H5	17:AY:58:Y5P:C5	2.32	0.59
28:Aj:90:ASP:OD1	33:Ap:215:ARG:NH2	2.27	0.59
65:BY:145:ARG:HH12	65:BY:157:PRO:HD3	1.66	0.59
73:Bh:216:ARG:NE	73:Bh:316:TYR:HD1	2.00	0.59
73:Bh:308:THR:HG22	73:Bh:310:ASN:H	1.67	0.59
79:Bn:74:ILE:O	79:Bn:81:ARG:NH1	2.34	0.59
20:Ab:87:LEU:HD22	24:Af:90:LEU:HG	1.83	0.59
24:Af:115:ILE:HD13	24:Af:141:VAL:HG21	1.83	0.59
32:Ao:656:UNK:HB1	32:Ao:674:UNK:HG1	1.85	0.59
33:Ap:108:CYS:SG	33:Ap:146:GLN:HG3	2.43	0.59
46:BA:58:C:C2'	46:BA:59:A:H5"	2.33	0.59
46:BA:1230:G:H4'	46:BA:1230:G:OP1	2.01	0.59
49:BE:128:HIS:CD2	49:BE:173:LYS:NZ	2.70	0.59
50:BF:276:HIS:O	77:Bl:90:ARG:NH2	2.35	0.59
55:BO:64:THR:HG22	55:BO:66:VAL:H	1.66	0.59
60:BT:79:GLU:HG2	60:BT:147:ALA:HB1	1.84	0.59
70:Be:51:ILE:HG22	70:Be:53:GLU:H	1.66	0.59
86:Bw:85:LYS:HE3	86:Bw:86:MET:HE3	1.84	0.59
1:AA:444:G:H5'	1:AA:445:C:OP2	2.03	0.59
22:Ad:50:PRO:HB2	33:Ap:213:LEU:HD22	1.84	0.59
25:Ag:178:ASP:N	25:Ag:178:ASP:OD1	2.35	0.59
38:B2:100:LEU:HB3	38:B2:144:LEU:HD11	1.85	0.59
46:BA:36:A:C4	70:Be:32:LYS:HG3	2.37	0.59
46:BA:747:C:N3	64:BX:54:ARG:HD3	2.17	0.59
49:BE:210:THR:OG1	49:BE:262:GLY:O	2.12	0.59
72:Bg:108:SER:HB3	72:Bg:110:LEU:H	1.67	0.59
88:Bz:17:UNK:HA	88:Bz:20:UNK:CG	2.29	0.59
19:Aa:312:UNK:HB1	19:Aa:333:UNK:CG	2.33	0.59
29:Ak:128:LEU:HG	32:Ao:74:LEU:HD21	1.85	0.59
32:Ao:220:UNK:HA	32:Ao:223:UNK:HG3	1.84	0.59
44:B8:113:ARG:NH1	56:BP:76:LEU:HA	2.18	0.59
56:BP:56:GLU:HG2	56:BP:62:ARG:HA	1.84	0.59
60:BT:196:GLU:H	60:BT:196:GLU:CD	2.09	0.59
19:Aa:344:UNK:HA	19:Aa:347:UNK:HG3	1.84	0.59
25:Ag:89:GLN:HE22	25:Ag:359:TYR:HE1	1.49	0.59
25:Ag:202:LYS:NZ	25:Ag:220:PRO:HD3	2.17	0.59
32:Ao:655:UNK:HG2	32:Ao:674:UNK:HB2	1.84	0.59
39:B3:38:ARG:HB2	46:BA:409:U:OP1	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:BP:138:VAL:O	56:BP:157:GLN:HG2	2.03	0.59
56:BP:261:ASP:HB2	56:BP:264:GLN:HB2	1.84	0.59
66:Ba:193:LEU:HD13	86:Bw:184:VAL:HA	1.85	0.59
88:Bz:308:UNK:HA	88:Bz:311:UNK:HG3	1.85	0.59
1:AA:77:G:H8	1:AA:77:G:OP2	1.84	0.59
7:AI:207:GLU:HG3	7:AI:212:GLU:O	2.03	0.59
25:Ag:215:THR:HG23	25:Ag:219:ARG:HG3	1.85	0.59
32:Ao:203:UNK:HG2	32:Ao:204:UNK:N	2.17	0.59
46:BA:622:A:P	56:BP:34:ARG:HH22	2.25	0.59
46:BA:1306:A:H5'	57:BQ:184:PRO:HA	1.83	0.59
50:BF:287:ARG:HD2	85:Bv:33:ARG:NH1	2.17	0.59
55:BO:52:HIS:CD2	55:BO:53:ARG:HG3	2.38	0.59
62:BV:104:HIS:HB2	62:BV:138:LEU:HD11	1.84	0.59
68:Bc:116:LEU:HD11	68:Bc:122:ILE:HD11	1.85	0.59
82:Bq:106:LYS:HE3	82:Bq:108:GLU:HB2	1.83	0.59
84:Bu:75:ARG:HH12	84:Bu:108:ASP:CG	2.11	0.59
88:Bz:15:UNK:O	88:Bz:18:UNK:HG3	2.03	0.59
4:AE:308:GLN:HG3	4:AE:312:TYR:CD1	2.38	0.59
12:AO:153:HIS:HA	12:AO:156:PHE:HD2	1.67	0.59
13:AP:105:THR:HG21	22:Ad:56:LEU:HD11	1.84	0.59
17:AV:55:Y5P:O2'	17:AV:57:Y5P:C5	2.51	0.59
19:Aa:315:UNK:CG	19:Aa:316:UNK:N	2.66	0.59
20:Ab:94:SER:OG	20:Ab:95:THR:N	2.34	0.59
23:Ae:38:UNK:HA	23:Ae:41:UNK:HG3	1.84	0.59
23:Ae:204:UNK:HB1	23:Ae:223:UNK:CG	2.32	0.59
23:Ae:267:UNK:HG2	23:Ae:270:UNK:CG	2.26	0.59
44:B8:168:ARG:NE	46:BA:225:U:OP1	2.21	0.59
57:BQ:106:ARG:HB3	57:BQ:106:ARG:HH11	1.67	0.59
68:Bc:45:PHE:HD2	68:Bc:253:ARG:NH1	2.00	0.59
72:Bg:34:SER:OG	72:Bg:70:CYS:O	2.20	0.59
80:Bo:101:GLU:O	80:Bo:105:LYS:HG2	2.03	0.59
83:Bt:55:THR:HG22	83:Bt:56:ALA:H	1.67	0.59
5:AF:10:LEU:HD23	5:AF:88:VAL:HA	1.84	0.59
10:AL:136:GLN:CD	10:AL:136:GLN:H	2.11	0.59
19:Aa:341:UNK:O	19:Aa:345:UNK:HG3	2.02	0.59
25:Ag:386:ASN:HD22	25:Ag:389:GLN:H	1.49	0.59
29:Ak:300:SER:O	29:Ak:304:GLU:HB3	2.03	0.59
32:Ao:197:UNK:O	32:Ao:234:UNK:HG1	2.03	0.59
33:Ap:91:ARG:NH2	33:Ap:103:ASN:O	2.36	0.59
46:BA:329:A:H2'	46:BA:329:A:N3	2.17	0.59
46:BA:743:A:OP2	70:Be:44:ARG:NH2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:BF:76:ARG:NH1	78:Bm:112:ALA:HB2	2.17	0.59
56:BP:183:SER:HA	56:BP:186:ILE:HD12	1.85	0.59
60:BT:79:GLU:OE2	60:BT:140:ARG:NH2	2.36	0.59
60:BT:138:ILE:HA	60:BT:187:LEU:HD12	1.84	0.59
69:Bd:97:LYS:HA	69:Bd:99:ARG:HH11	1.67	0.59
4:AE:162:LYS:O	4:AE:166:GLU:HG2	2.03	0.59
6:AG:139:ARG:NH2	25:Ag:363:ASN:OD1	2.36	0.59
10:AL:127:ARG:HD2	10:AL:132:CYS:HB3	1.85	0.59
11:AN:33:LYS:HB3	11:AN:90:ARG:CZ	2.33	0.59
13:AP:34:ILE:HG22	13:AP:51:LEU:HB2	1.83	0.59
19:Aa:240:GLU:HA	19:Aa:243:LYS:HB2	1.84	0.59
23:Ae:63:UNK:HG2	23:Ae:65:UNK:HG3	1.80	0.59
23:Ae:118:UNK:C	23:Ae:119:UNK:HG3	2.32	0.59
23:Ae:142:UNK:O	23:Ae:146:UNK:HG2	2.02	0.59
23:Ae:390:UNK:C	23:Ae:393:UNK:HG3	2.33	0.59
24:Af:117:PHE:HB3	24:Af:143:LEU:HD12	1.84	0.59
32:Ao:366:UNK:HG1	32:Ao:400:UNK:CG	2.32	0.59
32:Ao:535:UNK:HG2	32:Ao:554:UNK:CG	2.31	0.59
32:Ao:671:UNK:CA	32:Ao:674:UNK:HG3	2.33	0.59
49:BE:128:HIS:CD2	49:BE:173:LYS:HZ1	2.21	0.59
56:BP:216:ASP:HB3	56:BP:218:LYS:HB2	1.85	0.59
57:BQ:33:LEU:HD22	82:Bq:125:ASN:HD22	1.68	0.59
62:BV:117:LEU:HD13	62:BV:198:ARG:HH11	1.67	0.59
17:AV:59:Y5P:H4A	17:AV:60:Y5P:C4	2.31	0.58
19:Aa:300:VAL:HG11	19:Aa:330:UNK:HG1	1.85	0.58
25:Ag:383:SER:HB3	25:Ag:393:LEU:HD12	1.85	0.58
32:Ao:324:UNK:HA	32:Ao:327:UNK:HG3	1.85	0.58
32:Ao:366:UNK:CG	32:Ao:400:UNK:HG2	2.33	0.58
32:Ao:420:UNK:CB	32:Ao:459:UNK:HG1	2.26	0.58
45:B9:96:LYS:NZ	46:BA:1511:U:OP1	2.33	0.58
46:BA:1255:A:H3'	46:BA:1255:A:C8	2.38	0.58
49:BE:197:HIS:CD2	49:BE:318:THR:HG22	2.37	0.58
75:Bj:53:LEU:HG	75:Bj:238:LEU:HD11	1.85	0.58
86:Bw:206:ARG:HB3	86:Bw:225:TYR:HE1	1.68	0.58
4:AE:358:THR:HG22	4:AE:360:GLN:H	1.67	0.58
7:AI:276:LYS:HG3	7:AI:281:LYS:HG2	1.85	0.58
23:Ae:113:UNK:O	23:Ae:117:UNK:HG3	2.03	0.58
25:Ag:205:GLU:OE2	25:Ag:248:ARG:NH1	2.37	0.58
32:Ao:521:UNK:HA	32:Ao:524:UNK:HG3	1.84	0.58
40:B4:72:PRO:HG2	75:Bj:87:HIS:CD2	2.38	0.58
46:BA:101:U:O2'	46:BA:102:G:O4'	2.20	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:BY:126:THR:HB	65:BY:152:ARG:NH1	2.18	0.58
4:AE:279:LEU:O	20:Ab:4:SER:OG	2.18	0.58
12:AO:174:THR:HB	14:AQ:101:ALA:HB1	1.86	0.58
22:Ad:77:GLU:O	22:Ad:81:LYS:HG2	2.04	0.58
23:Ae:46:UNK:HG1	23:Ae:77:UNK:HG1	1.69	0.58
23:Ae:359:UNK:O	23:Ae:363:UNK:HG3	2.04	0.58
33:Ap:95:ILE:HG13	33:Ap:145:LYS:NZ	2.18	0.58
46:BA:218:A:P	56:BP:109:ARG:HH22	2.27	0.58
46:BA:704:A:OP1	64:BX:50:ARG:NH2	2.28	0.58
46:BA:1161:A:H5"	46:BA:1162:G:OP2	2.04	0.58
46:BA:1205:C:H5'	46:BA:1206:A:OP2	2.03	0.58
49:BE:95:SER:HB2	49:BE:303:LYS:HZ1	1.68	0.58
53:BK:19:MET:HG2	53:BK:71:PHE:HD1	1.68	0.58
54:BN:81:THR:HB	54:BN:83:TYR:HD2	1.69	0.58
58:BR:149:LEU:HD21	68:Bc:296:LEU:HD11	1.84	0.58
64:BX:7:TYR:HD2	70:Be:37:LYS:HE3	1.68	0.58
73:Bh:59:ARG:NH1	73:Bh:181:SER:O	2.35	0.58
78:Bm:92:LEU:N	78:Bm:122:CYS:O	2.29	0.58
2:AB:79:SER:OG	2:AB:80:VAL:N	2.35	0.58
32:Ao:171:UNK:HA	32:Ao:174:UNK:HG3	1.84	0.58
32:Ao:535:UNK:HA	32:Ao:538:UNK:HG3	1.85	0.58
46:BA:131:G:O2'	65:BY:40:ARG:O	2.16	0.58
46:BA:686:A:H3'	46:BA:687:A:H4'	1.86	0.58
46:BA:971:A:N3	92:BA:1958:HOH:O	2.32	0.58
53:BK:66:LEU:HA	53:BK:85:PRO:HA	1.85	0.58
54:BN:20:LEU:HB2	54:BN:141:LEU:HD22	1.84	0.58
61:BU:149:ARG:HD2	71:Bf:56:ARG:HH21	1.68	0.58
88:Bz:9:UNK:HA	88:Bz:12:UNK:HG3	1.84	0.58
1:AA:885:U:C5	23:Ae:102:UNK:HG3	2.39	0.58
23:Ae:401:UNK:O	23:Ae:405:UNK:HG3	2.04	0.58
42:B6:18:VAL:HG21	42:B6:58:GLU:HG3	1.84	0.58
46:BA:450:U:O2'	46:BA:1171:A:N3	2.36	0.58
71:Bf:50:ALA:HB3	71:Bf:59:VAL:HG22	1.85	0.58
1:AA:174:C:H2'	1:AA:175:A:O4'	2.04	0.58
10:AL:76:ALA:HB3	10:AL:78:ARG:HE	1.68	0.58
21:Ac:24:LYS:NZ	21:Ac:106:LEU:HA	2.18	0.58
23:Ae:118:UNK:O	23:Ae:119:UNK:HG3	2.04	0.58
25:Ag:153:HIS:HD2	25:Ag:260:ALA:HB3	1.68	0.58
28:Aj:78:ARG:HH21	28:Aj:144:LYS:HE3	1.69	0.58
59:BS:44:VAL:HG12	67:Bb:225:LEU:HD13	1.84	0.58
61:BU:23:GLU:HA	61:BU:26:LYS:HE3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:Bw:213:ARG:HB2	86:Bw:213:ARG:HH11	1.66	0.58
86:Bw:226:GLN:HE22	86:Bw:275:THR:H	1.51	0.58
1:AA:225:A:N1	1:AA:272:A:O2'	2.37	0.58
1:AA:320:A:N6	1:AA:390:A:H1'	2.19	0.58
3:AC:72:HIS:HD2	3:AC:74:GLY:H	1.51	0.58
4:AE:148:LEU:HD11	32:Ao:109:ALA:HB2	1.85	0.58
38:B2:123:ARG:HH22	64:BX:30:ARG:HG2	1.68	0.58
46:BA:841:C:OP1	48:BD:264:ASN:ND2	2.37	0.58
60:BT:165:GLU:HB2	60:BT:168:ASN:HB2	1.85	0.58
65:BY:195:GLU:OE1	65:BY:195:GLU:N	2.37	0.58
75:Bj:63:LEU:HB2	75:Bj:68:GLU:HG2	1.85	0.58
86:Bw:128:GLU:O	86:Bw:130:THR:N	2.35	0.58
86:Bw:141:CYS:SG	86:Bw:404:VAL:HG21	2.44	0.58
2:AB:123:HIS:NE2	20:Ab:41:LEU:HD12	2.18	0.58
32:Ao:157:UNK:HG1	32:Ao:173:UNK:O	2.03	0.58
46:BA:664:G:H2'	46:BA:665:C:C6	2.37	0.58
49:BE:292:HIS:CE1	49:BE:295:CYS:HB3	2.39	0.58
59:BS:41:ASN:HB3	67:Bb:293:LEU:HD12	1.86	0.58
63:BW:151:LEU:HB2	63:BW:167:LYS:HB2	1.86	0.58
65:BY:189:PRO:O	70:Be:93:THR:OG1	2.16	0.58
67:Bb:265:PHE:HZ	67:Bb:322:ARG:HH11	1.49	0.58
68:Bc:78:MET:HE2	68:Bc:83:SER:HB3	1.85	0.58
73:Bh:242:VAL:HG12	73:Bh:246:LYS:HE3	1.85	0.58
28:Aj:83:LYS:HG3	28:Aj:140:ARG:HH21	1.69	0.58
32:Ao:315:UNK:HA	32:Ao:318:UNK:HG3	1.84	0.58
44:B8:183:ARG:NH1	67:Bb:354:GLN:HE21	2.01	0.58
46:BA:1025:G:OP2	46:BA:1276:C:H5'	2.04	0.58
64:BX:71:ARG:HG2	64:BX:71:ARG:HH11	1.68	0.58
1:AA:707:A:H3'	1:AA:708:A:C5'	2.31	0.58
7:AI:170:LEU:HD11	7:AI:174:LYS:HE3	1.84	0.58
12:AO:116:VAL:O	12:AO:181:LYS:NZ	2.28	0.58
14:AQ:33:LEU:HD12	21:Ac:56:GLN:HE21	1.69	0.58
23:Ae:222:UNK:HG1	23:Ae:299:UNK:CG	2.33	0.58
46:BA:224:C:H5'	56:BP:133:LYS:HE3	1.84	0.58
49:BE:96:ARG:NH2	49:BE:197:HIS:O	2.37	0.58
67:Bb:268:PHE:HB2	67:Bb:319:PHE:CE1	2.38	0.58
77:Bl:142:GLU:HB3	83:Bt:88:LEU:HD13	1.85	0.58
25:Ag:106:GLU:OE2	29:Ak:315:LYS:NZ	2.26	0.57
26:Ah:379:LEU:HB3	26:Ah:386:LEU:HB2	1.86	0.57
32:Ao:235:UNK:HG1	32:Ao:237:UNK:CB	2.33	0.57
32:Ao:299:UNK:O	32:Ao:303:UNK:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:Ao:497:UNK:C	32:Ao:500:UNK:HG3	2.34	0.57
46:BA:178:U:O2'	46:BA:188:A:O4'	2.18	0.57
46:BA:1546:A:H5'	46:BA:1547:A:OP2	2.03	0.57
48:BD:157:ASN:HB2	48:BD:179:GLU:OE2	2.04	0.57
49:BE:99:LEU:HD12	49:BE:198:PHE:HE1	1.68	0.57
56:BP:100:ARG:HH21	56:BP:126:GLY:HA2	1.69	0.57
1:AA:641:A:H2'	1:AA:642:G:H8	1.67	0.57
3:AC:100:PHE:HE2	3:AC:155:LEU:HD21	1.69	0.57
4:AE:286:GLU:HB3	4:AE:288:HIS:CE1	2.39	0.57
23:Ae:197:UNK:CG	23:Ae:230:UNK:CG	2.72	0.57
23:Ae:227:UNK:HA	23:Ae:230:UNK:HB1	1.86	0.57
29:Ak:55:LEU:O	32:Ao:93:PRO:HB3	2.04	0.57
32:Ao:161:UNK:O	32:Ao:165:UNK:CG	2.43	0.57
32:Ao:371:UNK:HG2	32:Ao:372:UNK:N	2.20	0.57
41:B5:140:GLN:NE2	41:B5:176:GLU:O	2.36	0.57
46:BA:616:A:H8	72:Bg:71:CYS:HB2	1.69	0.57
46:BA:1199:A:H61	56:BP:71:GLN:HE22	1.51	0.57
55:BO:87:VAL:HG13	55:BO:123:ILE:HG12	1.85	0.57
84:Bu:52:SER:HB2	84:Bu:57:THR:HG21	1.86	0.57
84:Bu:103:HIS:HB3	84:Bu:106:SER:HB3	1.86	0.57
1:AA:641:A:H2'	1:AA:642:G:C8	2.39	0.57
4:AE:288:HIS:HD2	4:AE:289:THR:H	1.52	0.57
6:AG:152:CYS:SG	6:AG:219:VAL:HB	2.44	0.57
14:AQ:103:THR:HG23	21:Ac:35:ASN:HD21	1.69	0.57
25:Ag:310:SER:O	25:Ag:314:SER:OG	2.21	0.57
32:Ao:175:UNK:C	32:Ao:178:UNK:HG3	2.35	0.57
32:Ao:301:UNK:HA	32:Ao:304:UNK:HG3	1.86	0.57
46:BA:1293:G:H2'	46:BA:1296:C:H42	1.68	0.57
46:BA:1546:A:C2	49:BE:176:VAL:HG21	2.39	0.57
50:BF:211:ARG:NH1	78:Bm:59:ARG:HD2	2.19	0.57
54:BN:58:VAL:HG22	54:BN:126:HIS:HB2	1.85	0.57
59:BS:178:ILE:HD11	84:Bu:176:ARG:NH1	2.15	0.57
65:BY:212:LYS:HZ3	65:BY:214:TYR:HE1	1.50	0.57
73:Bh:121:ASP:N	73:Bh:121:ASP:OD1	2.38	0.57
75:Bj:99:ALA:HA	75:Bj:102:LYS:HD2	1.86	0.57
1:AA:202:A:N1	28:Aj:53:ARG:NH2	2.51	0.57
1:AA:630:A:H2'	1:AA:631:A:H8	1.68	0.57
3:AC:50:PRO:HB3	3:AC:167:ILE:HD11	1.86	0.57
4:AE:288:HIS:CD2	4:AE:289:THR:H	2.22	0.57
4:AE:292:HIS:HE1	4:AE:357:GLU:H	1.52	0.57
23:Ae:196:UNK:O	23:Ae:200:UNK:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:62:C:O2'	1:AA:198:C:H5'	2.04	0.57
1:AA:196:A:P	13:AP:20:ARG:HH11	2.28	0.57
1:AA:327:U:O2'	1:AA:328:A:N7	2.35	0.57
3:AC:69:LEU:HD23	29:Ak:109:LYS:HE2	1.85	0.57
15:AR:50:ASP:HA	24:Af:86:ARG:NH1	2.19	0.57
19:Aa:142:ALA:HB2	28:Aj:168:PRO:HB3	1.87	0.57
31:An:144:ARG:HH11	31:An:144:ARG:HA	1.69	0.57
46:BA:1565:G:O5'	49:BE:174:GLN:NE2	2.38	0.57
47:BB:24:P5P:H4'	59:BS:108:ARG:HH11	1.69	0.57
48:BD:198:GLU:OE2	48:BD:202:GLY:N	2.37	0.57
59:BS:39:VAL:HG12	59:BS:41:ASN:H	1.69	0.57
66:Ba:151:ASP:N	66:Ba:151:ASP:OD1	2.38	0.57
1:AA:881:A:N3	23:Ae:66:UNK:HG1	2.19	0.57
25:Ag:59:UNK:HG2	25:Ag:62:UNK:HB2	1.86	0.57
29:Ak:194:LYS:NZ	29:Ak:245:LYS:NZ	2.53	0.57
32:Ao:605:UNK:HG1	32:Ao:651:UNK:HG2	1.86	0.57
36:B0:119:ARG:NH1	76:Bk:65:ALA:HB2	2.20	0.57
38:B2:127:PRO:HD3	74:Bi:66:VAL:HB	1.87	0.57
41:B5:141:MET:HB2	41:B5:173:ARG:NH2	2.19	0.57
1:AA:14:C:OP2	4:AE:226:ARG:NH2	2.37	0.57
1:AA:561:U:H1'	1:AA:711:A:N6	2.19	0.57
3:AC:112:ARG:HB2	3:AC:112:ARG:NH1	2.20	0.57
4:AE:198:TRP:HB2	4:AE:225:VAL:CG1	2.35	0.57
7:AI:255:UNK:HG1	7:AI:371:LEU:CD1	2.31	0.57
23:Ae:232:UNK:CG	23:Ae:235:UNK:HG3	2.31	0.57
26:Ah:352:LYS:O	26:Ah:354:PRO:HD3	2.04	0.57
46:BA:1074:A:H2'	46:BA:1075:A:C8	2.39	0.57
1:AA:956:G:H2'	1:AA:957:A:C8	2.40	0.57
4:AE:323:ILE:HD13	4:AE:350:PHE:CE1	2.39	0.57
9:AK:112:ALA:HB3	9:AK:137:ALA:HB2	1.85	0.57
18:AX:21:Y5P:H4A	18:AX:22:Y5P:H4	1.87	0.57
23:Ae:56:UNK:O	23:Ae:60:UNK:HG2	2.04	0.57
23:Ae:75:UNK:CG	23:Ae:91:UNK:HG1	2.35	0.57
25:Ag:209:TRP:CZ3	25:Ag:215:THR:HB	2.38	0.57
32:Ao:342:UNK:O	32:Ao:346:UNK:HB1	2.04	0.57
32:Ao:344:UNK:HG2	32:Ao:345:UNK:N	2.19	0.57
36:B0:100:THR:HG22	36:B0:102:GLU:HG3	1.85	0.57
53:BK:54:ASN:HB3	53:BK:58:LYS:HE3	1.85	0.57
67:Bb:92:LEU:HD12	67:Bb:170:ARG:HB2	1.87	0.57
4:AE:369:HIS:HE1	4:AE:391:LEU:HD22	1.69	0.57
7:AI:275:GLY:H	7:AI:348:ALA:HB2	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Ae:200:UNK:HG1	23:Ae:226:UNK:HG1	1.86	0.57
32:Ao:160:UNK:O	32:Ao:164:UNK:HG3	2.05	0.57
38:B2:88:THR:HG22	38:B2:90:GLN:H	1.69	0.57
43:B7:75:THR:HG23	43:B7:78:GLY:H	1.70	0.57
45:B9:83:GLY:H	46:BA:1525:U:C5'	2.17	0.57
46:BA:341:C:H2'	46:BA:342:C:C6	2.39	0.57
46:BA:558:A:O2'	46:BA:559:C:OP1	2.20	0.57
46:BA:664:G:H5"	46:BA:777:G:O2'	2.04	0.57
56:BP:47:ARG:NH1	62:BV:183:ASN:HB2	2.20	0.57
60:BT:99:MET:HE3	60:BT:167:TYR:CZ	2.40	0.57
66:Ba:358:GLN:HE21	66:Ba:360:ASN:HD21	1.51	0.57
76:Bk:92:ASN:HD22	76:Bk:189:HIS:HA	1.70	0.57
1:AA:28:U:H2'	1:AA:29:A:H8	1.70	0.57
1:AA:344:G:H1	9:AK:121:ASN:HB2	1.70	0.57
24:Af:135:TYR:HA	24:Af:139:THR:HG21	1.87	0.57
25:Ag:211:LYS:HE3	25:Ag:212:ARG:HE	1.69	0.57
32:Ao:160:UNK:HA	32:Ao:163:UNK:CG	2.33	0.57
36:B0:65:ASN:N	36:B0:65:ASN:OD1	2.37	0.57
46:BA:1476:U:H2'	46:BA:1477:G:H8	1.70	0.57
61:BU:93:CYS:O	62:BV:150:LYS:HE2	2.04	0.57
62:BV:98:ARG:HH11	62:BV:113:THR:CG2	2.18	0.57
65:BY:131:THR:HG21	65:BY:147:SER:HB3	1.87	0.57
68:Bc:52:GLN:HG3	68:Bc:216:LEU:HD11	1.87	0.57
4:AE:261:ALA:HB2	4:AE:270:LYS:NZ	2.20	0.56
13:AP:20:ARG:NH2	13:AP:38:HIS:O	2.38	0.56
15:AR:65:LYS:HD3	15:AR:69:CYS:HB3	1.88	0.56
15:AR:73:VAL:HG22	15:AR:80:LEU:HD21	1.87	0.56
16:AU:52:ARG:HH11	16:AU:52:ARG:CB	2.14	0.56
17:AY:67:Y5P:C4	17:AY:68:Y5P:H4	2.34	0.56
23:Ae:54:UNK:O	23:Ae:58:UNK:HG2	2.05	0.56
23:Ae:90:UNK:CG	23:Ae:91:UNK:N	2.68	0.56
32:Ao:197:UNK:CG	32:Ao:230:UNK:HG2	2.28	0.56
44:B8:172:TYR:HB2	44:B8:175:ASP:HB2	1.86	0.56
46:BA:1386:A:H5'	46:BA:1387:A:OP2	2.05	0.56
50:BF:107:LYS:HA	79:Bn:74:ILE:HD12	1.87	0.56
50:BF:244:PRO:HB2	50:BF:246:VAL:HG23	1.86	0.56
66:Ba:136:VAL:HG11	66:Ba:417:LEU:HD23	1.86	0.56
74:Bi:235:GLN:HB2	74:Bi:238:VAL:HG12	1.86	0.56
86:Bw:89:MET:HA	86:Bw:271:GLN:HB3	1.86	0.56
88:Bz:409:UNK:C	88:Bz:412:UNK:HG3	2.34	0.56
1:AA:15:C:O2'	1:AA:293:A:N1	2.29	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AK:68:ILE:HG22	9:AK:70:GLY:H	1.71	0.56
26:Ah:301:LYS:HD3	32:Ao:140:LEU:HD11	1.88	0.56
29:Ak:199:ARG:H	29:Ak:199:ARG:HD2	1.69	0.56
32:Ao:320:UNK:O	32:Ao:323:UNK:HG3	2.04	0.56
32:Ao:424:UNK:HA	32:Ao:427:UNK:HG3	1.86	0.56
64:BX:37:GLU:HB3	64:BX:104:THR:HG23	1.87	0.56
72:Bg:28:ARG:NH1	72:Bg:28:ARG:HB3	2.20	0.56
80:Bo:48:ASP:OD1	80:Bo:48:ASP:N	2.36	0.56
88:Bz:302:UNK:HG2	88:Bz:303:UNK:N	2.19	0.56
1:AA:641:A:N7	4:AE:260:LYS:NZ	2.53	0.56
1:AA:891:C:H4'	1:AA:891:C:OP1	2.04	0.56
4:AE:290:ILE:HG13	4:AE:307:LYS:HB2	1.87	0.56
17:AY:9:Y5P:H4	17:AY:22:Y5P:H5	1.87	0.56
17:AY:36:P5P:C6	17:AY:37:Y5P:H4	2.34	0.56
19:Aa:194:VAL:HG22	19:Aa:203:ILE:HD13	1.86	0.56
21:Ac:32:VAL:HG21	21:Ac:52:ILE:HD11	1.87	0.56
23:Ae:212:UNK:O	23:Ae:215:UNK:HG3	2.05	0.56
24:Af:96:ALA:HB1	24:Af:145:LEU:HD23	1.87	0.56
25:Ag:57:UNK:CG	25:Ag:142:HIS:NE2	2.68	0.56
25:Ag:57:UNK:HG2	25:Ag:142:HIS:NE2	2.21	0.56
32:Ao:671:UNK:HA	32:Ao:674:UNK:CG	2.33	0.56
37:B1:87:LEU:HD23	37:B1:104:VAL:HB	1.86	0.56
46:BA:39:A:H4'	46:BA:40:C:OP1	2.06	0.56
46:BA:472:G:H3'	46:BA:472:G:N3	2.20	0.56
46:BA:526:U:O2'	46:BA:527:G:O4'	2.21	0.56
46:BA:664:G:H2'	46:BA:665:C:H6	1.70	0.56
46:BA:892:U:O2'	48:BD:285:ARG:O	2.20	0.56
50:BF:290:TYR:CE1	77:Bl:53:PRO:HG2	2.40	0.56
52:BJ:101:HIS:CE1	52:BJ:109:LYS:NZ	2.73	0.56
55:BO:58:ILE:HD11	55:BO:76:ALA:HB2	1.87	0.56
60:BT:103:ARG:NH1	60:BT:108:ILE:HB	2.21	0.56
72:Bg:31:PHE:HB2	72:Bg:65:VAL:HG13	1.87	0.56
73:Bh:105:ARG:HD2	73:Bh:112:LYS:HB2	1.86	0.56
88:Bz:417:UNK:HG2	88:Bz:418:UNK:N	2.20	0.56
1:AA:844:C:H5'	18:AX:18:Y5P:H4A	1.87	0.56
2:AB:81:ARG:HA	24:Af:84:MET:HE1	1.86	0.56
3:AC:154:HIS:CG	29:Ak:77:PRO:HG3	2.40	0.56
7:AI:263:UNK:HG2	7:AI:265:UNK:HG3	1.86	0.56
23:Ae:246:UNK:HG1	23:Ae:272:UNK:HG1	1.87	0.56
23:Ae:278:UNK:HA	23:Ae:281:UNK:HG3	1.87	0.56
32:Ao:507:UNK:HA	32:Ao:510:UNK:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:B0:90:TYR:HE1	36:B0:92:LEU:HD21	1.71	0.56
46:BA:174:C:OP1	54:BN:115:ASN:HB2	2.05	0.56
48:BD:111:ARG:NH1	48:BD:111:ARG:HG3	2.20	0.56
55:BO:77:ILE:HD11	55:BO:107:LEU:HD21	1.87	0.56
57:BQ:72:ILE:HD11	57:BQ:96:TYR:CE1	2.41	0.56
58:BR:139:ARG:HH11	58:BR:139:ARG:HG3	1.71	0.56
66:Ba:144:ARG:C	66:Ba:194:LYS:HZ3	2.12	0.56
67:Bb:47:ARG:NE	76:Bk:120:LYS:HZ1	1.83	0.56
68:Bc:186:LEU:HG	68:Bc:189:TRP:HE1	1.70	0.56
71:Bf:81:UNK:O	71:Bf:81:UNK:HG2	2.04	0.56
86:Bw:204:TRP:HZ3	86:Bw:227:ILE:HG13	1.70	0.56
23:Ae:185:UNK:O	23:Ae:189:UNK:HG2	2.06	0.56
23:Ae:222:UNK:C	23:Ae:225:UNK:HG3	2.33	0.56
23:Ae:254:UNK:HA	23:Ae:257:UNK:HG3	1.86	0.56
35:Az:702:UNK:C	35:Az:705:UNK:HG3	2.35	0.56
45:B9:98:ARG:HH12	46:BA:1360:U:H4'	1.70	0.56
46:BA:115:U:H3'	46:BA:116:A:H5"	1.86	0.56
46:BA:478:A:C2	63:BW:208:HIS:HA	2.40	0.56
50:BF:204:ILE:HD11	50:BF:237:LEU:HD21	1.87	0.56
50:BF:290:TYR:HB2	50:BF:293:PHE:HB3	1.87	0.56
61:BU:50:PHE:O	61:BU:53:CYS:HB3	2.05	0.56
63:BW:47:ARG:NH1	63:BW:76:ARG:HD2	2.20	0.56
86:Bw:51:LEU:HD23	86:Bw:61:ARG:NH1	2.20	0.56
87:Bx:148:ASN:OD1	87:Bx:148:ASN:N	2.36	0.56
1:AA:255:G:O6	10:AL:74:ASN:HB2	2.06	0.56
17:AV:31:Y5P:H4A	17:AV:32:Y5P:H4	1.87	0.56
36:B0:147:MET:HE3	67:Bb:338:ARG:HB2	1.87	0.56
47:BB:30:P5P:H2'	47:BB:31:Y5P:H6	1.87	0.56
59:BS:130:ARG:HH21	67:Bb:132:LEU:HD21	1.70	0.56
88:Bz:301:UNK:O	88:Bz:304:UNK:HG3	2.05	0.56
6:AG:155:VAL:H	6:AG:227:HIS:CE1	2.23	0.56
6:AG:240:ARG:NH2	30:Am:44:THR:O	2.38	0.56
17:AY:43:Y5P:OP1	17:AY:43:Y5P:HA	2.06	0.56
19:Aa:88:LYS:NZ	19:Aa:260:LEU:O	2.29	0.56
28:Aj:21:LEU:HD22	28:Aj:25:ARG:HH21	1.71	0.56
32:Ao:427:UNK:HG2	32:Ao:466:UNK:CG	2.35	0.56
38:B2:209:ARG:HG2	38:B2:209:ARG:HH11	1.71	0.56
38:B2:209:ARG:HG2	38:B2:209:ARG:NH1	2.21	0.56
46:BA:463:U:C6	87:Bx:168:ARG:NH1	2.74	0.56
46:BA:513:A:N7	46:BA:539:A:H4'	2.21	0.56
59:BS:41:ASN:ND2	67:Bb:292:GLN:OE1	2.27	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:BW:210:LEU:HD21	71:Bf:142:ARG:NH2	2.21	0.56
70:Be:44:ARG:NH1	86:Bw:157:ALA:HB3	2.04	0.56
76:Bk:162:LEU:HD21	76:Bk:167:ALA:HB2	1.87	0.56
78:Bm:70:ARG:O	78:Bm:73:SER:OG	2.15	0.56
88:Bz:417:UNK:O	88:Bz:420:UNK:CG	2.53	0.56
7:AI:373:ALA:O	7:AI:375:PRO:HD3	2.06	0.56
27:Ai:17:ARG:HH22	35:Az:698:UNK:HG3	1.67	0.56
32:Ao:280:UNK:HA	32:Ao:283:UNK:HG3	1.88	0.56
32:Ao:671:UNK:C	32:Ao:674:UNK:HG3	2.36	0.56
38:B2:139:ASP:O	38:B2:143:ALA:N	2.31	0.56
49:BE:195:ALA:H	49:BE:281:ASN:ND2	2.04	0.56
56:BP:26:ASN:HD22	83:Bt:95:LEU:HD22	1.71	0.56
59:BS:163:HIS:O	59:BS:167:GLU:HG2	2.06	0.56
67:Bb:92:LEU:HB2	67:Bb:170:ARG:HG3	1.88	0.56
67:Bb:258:PHE:HD1	67:Bb:258:PHE:H	1.54	0.56
72:Bg:28:ARG:HH21	73:Bh:177:GLN:NE2	2.02	0.56
82:Bq:110:LEU:HG	82:Bq:117:TYR:HB2	1.88	0.56
1:AA:248:C:OP1	10:AL:97:GLY:N	2.36	0.56
1:AA:881:A:H2'	23:Ae:66:UNK:HG2	1.88	0.56
5:AF:97:PRO:HG3	15:AR:76:LYS:NZ	2.21	0.56
7:AI:174:LYS:HA	24:Af:137:LYS:NZ	2.21	0.56
17:AV:2:Y5P:HA	36:B0:36:GLY:HA3	1.87	0.56
23:Ae:355:UNK:O	23:Ae:359:UNK:HG3	2.06	0.56
29:Ak:88:ARG:NH1	29:Ak:98:PRO:O	2.37	0.56
32:Ao:344:UNK:CG	32:Ao:345:UNK:N	2.68	0.56
46:BA:166:G:P	72:Bg:3:ALA:HB3	2.46	0.56
46:BA:478:A:H8	46:BA:478:A:OP1	1.89	0.56
46:BA:615:A:H1'	73:Bh:39:TYR:OH	2.06	0.56
48:BD:123:PHE:HB2	48:BD:166:ASN:HB2	1.87	0.56
59:BS:79:HIS:N	59:BS:174:GLU:OE2	2.37	0.56
63:BW:127:VAL:HG13	63:BW:132:VAL:O	2.06	0.56
88:Bz:606:UNK:C	88:Bz:609:UNK:HG3	2.35	0.56
1:AA:93:A:O2'	22:Ad:79:ARG:NH2	2.39	0.56
23:Ae:75:UNK:HG1	23:Ae:91:UNK:HG1	1.86	0.56
32:Ao:656:UNK:HB1	32:Ao:674:UNK:CG	2.36	0.56
49:BE:149:GLY:O	49:BE:173:LYS:HD2	2.06	0.56
70:Be:129:TYR:HB3	70:Be:130:PRO:HD3	1.87	0.56
73:Bh:184:PHE:O	73:Bh:186:VAL:HG23	2.06	0.56
86:Bw:163:ARG:HB2	86:Bw:301:LYS:HE2	1.88	0.56
1:AA:297:A:N6	1:AA:485:G:H4'	2.21	0.55
2:AB:161:CYS:O	2:AB:260:LYS:NZ	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AO:74:LEU:HB2	12:AO:77:TYR:HD2	1.70	0.55
13:AP:104:ILE:HG23	19:Aa:146:ILE:HD12	1.87	0.55
17:AY:8:Y5P:N3	17:AY:14:Y5P:C5	2.69	0.55
17:AY:55:Y5P:H5	17:AY:58:Y5P:C6	2.36	0.55
19:Aa:314:UNK:HA	19:Aa:317:UNK:CG	2.36	0.55
32:Ao:497:UNK:HA	32:Ao:500:UNK:HG3	1.88	0.55
46:BA:159:A:H61	54:BN:119:ARG:CB	2.19	0.55
46:BA:822:G:H5'	46:BA:823:C:OP2	2.06	0.55
46:BA:1546:A:H3'	46:BA:1547:A:H5'	1.88	0.55
56:BP:100:ARG:NH2	56:BP:126:GLY:HA2	2.21	0.55
61:BU:121:LYS:HD3	71:Bf:38:SER:HB3	1.88	0.55
69:Bd:158:HIS:O	69:Bd:162:THR:OG1	2.15	0.55
72:Bg:144:ARG:HB2	72:Bg:147:GLU:HB2	1.87	0.55
83:Bt:98:THR:O	83:Bt:100:LYS:HG2	2.04	0.55
88:Bz:404:UNK:HG2	88:Bz:405:UNK:N	2.21	0.55
1:AA:386:U:H5"	15:AR:114:ARG:HE	1.71	0.55
4:AE:197:THR:HG22	4:AE:199:GLY:H	1.71	0.55
9:AK:191:ARG:HH21	9:AK:194:ARG:HD3	1.71	0.55
37:B1:75:SER:HA	37:B1:80:TRP:CE2	2.41	0.55
43:B7:74:ARG:NH2	46:BA:31:A:O2'	2.39	0.55
46:BA:131:G:H8	46:BA:131:G:H5'	1.70	0.55
46:BA:277:A:H5'	46:BA:277:A:H8	1.71	0.55
46:BA:1519:U:H5	54:BN:177:ARG:HG3	1.71	0.55
50:BF:195:LEU:HD22	50:BF:202:TYR:HE2	1.71	0.55
56:BP:84:ASN:O	56:BP:87:HIS:HB3	2.07	0.55
87:Bx:108:CYS:SG	87:Bx:111:GLU:HB2	2.45	0.55
1:AA:12:G:H5'	4:AE:229:PHE:CD2	2.38	0.55
1:AA:44:U:H5'	1:AA:45:A:OP1	2.06	0.55
1:AA:344:G:N1	9:AK:121:ASN:HB2	2.22	0.55
1:AA:487:C:H5'	1:AA:488:A:OP2	2.06	0.55
15:AR:50:ASP:HA	24:Af:86:ARG:HH11	1.70	0.55
23:Ae:122:UNK:HG2	23:Ae:123:UNK:N	2.22	0.55
38:B2:156:ARG:O	38:B2:160:THR:N	2.38	0.55
46:BA:527:G:OP2	82:Bq:119:ARG:NH2	2.38	0.55
46:BA:616:A:C8	72:Bg:71:CYS:HB2	2.42	0.55
52:BJ:89:VAL:HG22	52:BJ:124:LYS:NZ	2.21	0.55
54:BN:20:LEU:HD22	54:BN:141:LEU:HD13	1.88	0.55
55:BO:69:VAL:HG23	55:BO:89:HIS:CE1	2.42	0.55
55:BO:128:ARG:NH1	60:BT:126:ALA:HA	2.21	0.55
56:BP:54:LYS:HG2	56:BP:59:ARG:HH22	1.72	0.55
66:Ba:153:ARG:HH11	66:Ba:187:LEU:CD2	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:Ba:329:TYR:HB3	66:Ba:334:LYS:NZ	2.21	0.55
86:Bw:326:LEU:O	86:Bw:330:THR:OG1	2.23	0.55
7:AI:294:ILE:HG12	7:AI:301:TYR:HB3	1.88	0.55
9:AK:80:LYS:HB3	9:AK:84:GLU:HB2	1.88	0.55
14:AQ:57:GLN:HE21	14:AQ:87:LYS:HZ3	1.53	0.55
23:Ae:69:UNK:HA	23:Ae:72:UNK:HG3	1.89	0.55
23:Ae:104:UNK:CG	23:Ae:107:UNK:CG	2.75	0.55
32:Ao:303:UNK:HG2	32:Ao:340:UNK:CG	2.36	0.55
46:BA:168:U:H4'	63:BW:207:THR:HG21	1.87	0.55
50:BF:60:ARG:NH1	78:Bm:122:CYS:SG	2.79	0.55
68:Bc:71:ASP:O	68:Bc:74:THR:OG1	2.17	0.55
69:Bd:164:ARG:HH22	76:Bk:91:LEU:HD21	1.71	0.55
71:Bf:90:UNK:HA	71:Bf:93:UNK:HG3	1.88	0.55
86:Bw:235:ILE:HB	86:Bw:290:HIS:HB3	1.89	0.55
86:Bw:310:CYS:HB3	86:Bw:313:GLN:HG3	1.88	0.55
1:AA:196:A:OP1	13:AP:20:ARG:NH1	2.38	0.55
6:AG:197:ARG:HH11	6:AG:197:ARG:CB	2.12	0.55
17:AV:37:Y5P:C4	17:AV:38:Y5P:H4	2.29	0.55
23:Ae:279:UNK:HG2	23:Ae:280:UNK:N	2.20	0.55
32:Ao:157:UNK:HB1	32:Ao:177:UNK:HG1	1.88	0.55
32:Ao:535:UNK:HG1	32:Ao:554:UNK:HG2	1.85	0.55
33:Ap:55:PRO:HB2	33:Ap:119:ASN:HB3	1.89	0.55
37:B1:238:LEU:HD21	70:Be:99:GLU:HG3	1.89	0.55
38:B2:230:ARG:HB3	38:B2:230:ARG:HH11	1.72	0.55
46:BA:342:C:H2'	46:BA:343:U:C6	2.42	0.55
46:BA:944:C:OP2	92:BA:1955:HOH:O	2.18	0.55
64:BX:64:PRO:HG2	64:BX:103:GLN:HE22	1.72	0.55
1:AA:287:C:N4	14:AQ:39:LEU:HA	2.22	0.55
1:AA:632:A:OP1	4:AE:269:ARG:NH2	2.39	0.55
9:AK:156:LEU:HD21	16:AU:36:ILE:HG23	1.89	0.55
28:Aj:6:VAL:O	28:Aj:7:ARG:HG2	2.05	0.55
46:BA:478:A:N1	63:BW:208:HIS:HA	2.21	0.55
56:BP:203:ARG:NH1	56:BP:264:GLN:O	2.40	0.55
60:BT:235:ARG:NH1	60:BT:260:TRP:CE2	2.75	0.55
67:Bb:169:PRO:HA	67:Bb:314:ALA:O	2.07	0.55
68:Bc:167:PRO:HG2	68:Bc:177:CYS:SG	2.47	0.55
1:AA:875:A:H62	28:Aj:17:ARG:NH1	2.04	0.55
4:AE:365:LYS:HG3	4:AE:366:LYS:HG2	1.88	0.55
5:AF:8:LEU:HB2	5:AF:64:PHE:HB2	1.86	0.55
5:AF:37:ARG:HA	22:Ad:167:PHE:HD1	1.71	0.55
23:Ae:109:UNK:HA	23:Ae:112:UNK:CG	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Ae:178:UNK:HG2	23:Ae:210:UNK:HB1	1.88	0.55
46:BA:128:A:C2	46:BA:129:A:C4	2.95	0.55
50:BF:97:HIS:CD2	56:BP:29:PRO:HB3	2.41	0.55
59:BS:151:TRP:CD1	59:BS:152:GLU:HG3	2.41	0.55
66:Ba:162:ARG:NH1	66:Ba:383:TYR:OH	2.40	0.55
67:Bb:209:ASP:OD1	67:Bb:209:ASP:N	2.38	0.55
68:Bc:140:TRP:CE3	68:Bc:176:PHE:HB3	2.42	0.55
68:Bc:156:LYS:HB3	68:Bc:159:TYR:CD2	2.41	0.55
1:AA:560:C:H42	1:AA:710:G:H1	1.54	0.55
1:AA:811:U:H5'	8:AJ:131:ARG:NH1	2.21	0.55
4:AE:150:ARG:HB2	4:AE:155:GLN:HE21	1.72	0.55
6:AG:155:VAL:HG13	30:Am:74:PHE:CZ	2.42	0.55
17:AY:24:Y5P:C4	17:AY:25:Y5P:H4	2.37	0.55
19:Aa:262:ARG:HE	19:Aa:267:PHE:HE2	1.54	0.55
19:Aa:314:UNK:O	19:Aa:317:UNK:HG3	2.06	0.55
23:Ae:120:UNK:CG	23:Ae:123:UNK:CG	2.85	0.55
29:Ak:106:GLU:OE2	29:Ak:109:LYS:NZ	2.40	0.55
32:Ao:521:UNK:HB1	32:Ao:534:UNK:HG1	1.87	0.55
46:BA:119:A:C6	46:BA:128:A:C8	2.95	0.55
50:BF:251:HIS:CE1	79:Bn:54:PHE:HD2	2.25	0.55
56:BP:208:GLU:HG2	85:Bv:99:MET:HE3	1.89	0.55
59:BS:52:ASN:HD21	59:BS:54:ARG:HB3	1.72	0.55
63:BW:77:GLN:H	63:BW:171:HIS:CD2	2.24	0.55
73:Bh:32:LYS:NZ	79:Bn:42:LYS:HZ3	2.03	0.55
14:AQ:96:THR:HB	14:AQ:98:LYS:NZ	2.20	0.55
19:Aa:310:UNK:HG3	19:Aa:313:UNK:HG1	1.88	0.55
23:Ae:35:UNK:HA	23:Ae:38:UNK:HG3	1.88	0.55
23:Ae:192:UNK:O	23:Ae:192:UNK:HG2	2.07	0.55
30:Am:62:ARG:HG3	30:Am:65:ALA:HB2	1.89	0.55
46:BA:545:A:H3'	46:BA:546:A:H5'	1.87	0.55
46:BA:1343:A:H2	46:BA:1364:A:N6	2.05	0.55
46:BA:1519:U:C5	54:BN:177:ARG:HG3	2.42	0.55
49:BE:96:ARG:HH11	49:BE:96:ARG:HB3	1.71	0.55
53:BK:67:PRO:HD2	53:BK:85:PRO:HA	1.88	0.55
65:BY:144:VAL:HG11	65:BY:153:ILE:HD12	1.89	0.55
68:Bc:300:VAL:HG23	68:Bc:301:HIS:CD2	2.41	0.55
71:Bf:84:UNK:HA	71:Bf:92:UNK:CG	2.37	0.55
4:AE:173:VAL:O	4:AE:177:GLU:HG2	2.07	0.55
5:AF:57:ARG:HH21	16:AU:3:ASN:HD22	1.55	0.55
37:B1:130:ARG:NH1	37:B1:134:LEU:HD11	2.22	0.55
46:BA:29:A:H2'	46:BA:30:U:O4'	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:BA:228:A:H4'	46:BA:229:G:H5'	1.89	0.55
46:BA:1141:U:H2'	46:BA:1142:U:H6	1.72	0.55
46:BA:1397:G:O2'	46:BA:1400:C:OP2	2.24	0.55
63:BW:81:SER:HA	63:BW:168:VAL:HG11	1.89	0.55
67:Bb:234:HIS:HE1	67:Bb:257:PRO:HA	1.72	0.55
72:Bg:56:ARG:HH11	72:Bg:56:ARG:HG3	1.71	0.55
76:Bk:106:TYR:OH	76:Bk:174:ILE:O	2.24	0.55
1:AA:838:A:C4	31:An:131:LEU:HD11	2.40	0.54
1:AA:885:U:C5	23:Ae:102:UNK:CG	2.90	0.54
8:AJ:132:VAL:HG21	11:AN:112:ARG:CZ	2.37	0.54
11:AN:29:TYR:HD2	11:AN:34:MET:HE3	1.72	0.54
19:Aa:227:LEU:O	19:Aa:231:VAL:HG23	2.08	0.54
19:Aa:334:UNK:HG2	19:Aa:334:UNK:O	2.05	0.54
22:Ad:65:GLN:HE21	28:Aj:193:LEU:HB3	1.72	0.54
29:Ak:194:LYS:HZ2	29:Ak:245:LYS:NZ	2.05	0.54
32:Ao:367:UNK:HG2	32:Ao:368:UNK:N	2.22	0.54
38:B2:101:HIS:HB2	65:BY:194:LEU:HD11	1.89	0.54
38:B2:123:ARG:HH12	64:BX:30:ARG:HB3	1.71	0.54
38:B2:125:ARG:NH1	74:Bi:62:LYS:O	2.39	0.54
46:BA:277:A:H5'	46:BA:277:A:C8	2.42	0.54
46:BA:567:C:OP2	83:Bt:9:ARG:HB3	2.07	0.54
59:BS:89:HIS:CD2	59:BS:119:THR:HG21	2.42	0.54
63:BW:113:GLN:O	63:BW:116:LYS:HB3	2.07	0.54
1:AA:647:A:H3'	1:AA:648:A:C5'	2.36	0.54
1:AA:717:G:OP1	7:AI:393:THR:OG1	2.26	0.54
4:AE:369:HIS:HA	4:AE:387:PRO:HD3	1.89	0.54
7:AI:161:LEU:HD11	7:AI:210:LEU:HD21	1.88	0.54
12:AO:69:PRO:HD2	12:AO:72:MET:SD	2.47	0.54
26:Ah:335:LYS:HA	26:Ah:340:ARG:HE	1.72	0.54
29:Ak:58:ARG:HB2	29:Ak:82:ALA:HA	1.89	0.54
31:An:146:LEU:HD12	31:An:149:ARG:NH1	2.23	0.54
32:Ao:537:UNK:O	32:Ao:541:UNK:CG	2.46	0.54
46:BA:163:A:H2'	61:BU:35:LYS:HZ1	1.72	0.54
46:BA:338:G:N3	46:BA:1065:G:O2'	2.39	0.54
46:BA:786:A:C2	58:BR:17:ARG:NH1	2.76	0.54
49:BE:239:ARG:HB3	49:BE:240:PRO:HD2	1.88	0.54
56:BP:26:ASN:OD1	56:BP:26:ASN:N	2.39	0.54
56:BP:105:ILE:HG23	56:BP:112:PRO:HD3	1.90	0.54
56:BP:138:VAL:H	56:BP:157:GLN:HE21	1.55	0.54
68:Bc:151:ILE:HA	68:Bc:199:PHE:HE1	1.72	0.54
32:Ao:265:UNK:HA	32:Ao:268:UNK:HG3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:Ao:581:UNK:HG2	32:Ao:658:UNK:HB1	1.88	0.54
46:BA:895:A:H2'	46:BA:896:C:H6	1.71	0.54
48:BD:247:ARG:HH12	48:BD:251:VAL:HG11	1.72	0.54
67:Bb:234:HIS:CE1	67:Bb:257:PRO:HA	2.42	0.54
68:Bc:173:ALA:HB1	68:Bc:320:VAL:HG11	1.88	0.54
84:Bu:152:LYS:O	84:Bu:156:MET:HG3	2.08	0.54
88:Bz:604:UNK:C	88:Bz:607:UNK:HG3	2.36	0.54
8:AJ:73:TYR:CE2	8:AJ:150:GLY:HA2	2.43	0.54
17:AY:68:Y5P:H4A	17:AY:69:Y5P:H4	1.88	0.54
22:Ad:58:GLU:O	22:Ad:62:GLN:HG2	2.07	0.54
22:Ad:117:HIS:O	22:Ad:121:LEU:HG	2.08	0.54
23:Ae:200:UNK:HB1	23:Ae:226:UNK:HG2	1.89	0.54
23:Ae:399:UNK:O	23:Ae:402:UNK:HG3	2.07	0.54
25:Ag:85:ARG:NH1	25:Ag:391:GLU:OE2	2.40	0.54
46:BA:122:G:H5'	46:BA:123:U:OP2	2.06	0.54
47:BB:26:Y5P:OP1	67:Bb:59:ARG:NH1	2.35	0.54
53:BK:95:ALA:HB1	53:BK:110:GLY:HA3	1.90	0.54
54:BN:80:HIS:HD2	54:BN:82:GLY:H	1.53	0.54
54:BN:91:THR:HB	54:BN:94:GLN:HG3	1.90	0.54
66:Ba:147:ILE:HG12	66:Ba:150:GLN:NE2	2.23	0.54
76:Bk:135:LEU:HD12	88:Bz:105:UNK:CG	2.33	0.54
86:Bw:399:ILE:HG23	86:Bw:404:VAL:HG13	1.89	0.54
1:AA:886:A:H5"	28:Aj:101:ARG:HG2	1.88	0.54
2:AB:223:ASP:OD1	2:AB:224:THR:N	2.37	0.54
4:AE:353:LEU:O	4:AE:356:GLN:HB2	2.07	0.54
23:Ae:207:UNK:HG1	23:Ae:219:UNK:HG2	1.90	0.54
23:Ae:394:UNK:O	23:Ae:398:UNK:HG3	2.08	0.54
32:Ao:190:UNK:HA	32:Ao:193:UNK:HG3	1.90	0.54
32:Ao:337:UNK:HG2	32:Ao:338:UNK:N	2.23	0.54
32:Ao:656:UNK:CB	32:Ao:674:UNK:HG1	2.38	0.54
46:BA:130:A:O2'	46:BA:131:G:H5"	2.08	0.54
46:BA:241:G:H2'	46:BA:350:A:H61	1.72	0.54
46:BA:403:C:C2'	46:BA:404:C:H5'	2.38	0.54
46:BA:432:G:H22	46:BA:457:A:H2	1.55	0.54
46:BA:981:U:H5'	46:BA:982:A:OP2	2.07	0.54
59:BS:130:ARG:HH11	67:Bb:129:ARG:HH11	1.54	0.54
62:BV:97:GLY:O	73:Bh:312:ARG:HA	2.06	0.54
83:Bt:24:PRO:HG2	87:Bx:169:TRP:HB2	1.90	0.54
84:Bu:142:GLN:HA	84:Bu:145:ASN:HD22	1.73	0.54
1:AA:482:U:H2'	1:AA:483:U:O4'	2.07	0.54
1:AA:635:C:H5'	2:AB:176:THR:HG21	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AK:67:PRO:HG2	9:AK:82:PHE:CD2	2.42	0.54
12:AO:144:MET:HE1	12:AO:150:ASP:HB3	1.89	0.54
19:Aa:342:UNK:HA	19:Aa:345:UNK:CG	2.38	0.54
21:Ac:34:TYR:HE2	21:Ac:66:MET:HB3	1.72	0.54
25:Ag:56:UNK:CG	25:Ag:146:LYS:HZ1	2.21	0.54
28:Aj:166:TYR:HD2	28:Aj:189:PRO:HB2	1.70	0.54
29:Ak:104:ASN:HD22	29:Ak:107:LEU:HD12	1.72	0.54
29:Ak:153:ILE:HG13	29:Ak:175:LEU:HD23	1.90	0.54
32:Ao:670:UNK:HA	32:Ao:673:UNK:HG3	1.88	0.54
46:BA:498:C:N4	46:BA:544:C:OP2	2.39	0.54
46:BA:1519:U:H3'	46:BA:1520:A:C5'	2.37	0.54
56:BP:47:ARG:HH11	62:BV:183:ASN:HB2	1.73	0.54
56:BP:77:ARG:NH1	56:BP:77:ARG:HB3	2.22	0.54
61:BU:65:ARG:NH1	61:BU:99:ARG:NH1	2.51	0.54
63:BW:95:MET:HE2	63:BW:99:GLN:HB3	1.90	0.54
66:Ba:216:GLU:O	66:Ba:218:ILE:HD12	2.08	0.54
67:Bb:179:VAL:HG13	67:Bb:197:GLU:HG3	1.88	0.54
69:Bd:165:ASP:OD2	75:Bj:185:ARG:NH2	2.40	0.54
12:AO:150:ASP:OD2	12:AO:153:HIS:HD2	1.91	0.54
13:AP:42:PRO:HG2	13:AP:45:GLY:HA3	1.90	0.54
15:AR:67:ILE:HD12	15:AR:136:VAL:HG13	1.90	0.54
23:Ae:68:UNK:CG	23:Ae:71:UNK:CG	2.85	0.54
23:Ae:106:UNK:HB1	23:Ae:383:UNK:HB1	1.89	0.54
26:Ah:335:LYS:O	26:Ah:340:ARG:HG3	2.08	0.54
33:Ap:104:PRO:HB2	33:Ap:109:ARG:HB3	1.90	0.54
41:B5:144:GLN:HE22	41:B5:175:ILE:HA	1.72	0.54
46:BA:60:U:C5	46:BA:61:U:H1'	2.43	0.54
46:BA:374:U:O2	46:BA:374:U:H2'	2.07	0.54
46:BA:403:C:H2'	46:BA:404:C:H5'	1.90	0.54
52:BJ:168:LEU:HD13	52:BJ:176:LEU:HB2	1.88	0.54
53:BK:19:MET:HE1	53:BK:69:LYS:HB3	1.88	0.54
59:BS:104:SER:OG	67:Bb:150:ARG:NH2	2.37	0.54
66:Ba:288:PRO:HD2	66:Ba:324:GLN:CD	2.32	0.54
84:Bu:101:ARG:HH12	84:Bu:131:GLU:HG3	1.71	0.54
1:AA:300:G:O2'	12:AO:159:MET:HE1	2.08	0.54
1:AA:885:U:C4	23:Ae:102:UNK:HG3	2.43	0.54
6:AG:199:VAL:HG11	6:AG:204:LYS:HD3	1.90	0.54
13:AP:67:ALA:HB1	19:Aa:160:ILE:HD12	1.88	0.54
16:AU:51:ARG:HG3	16:AU:54:ARG:HH12	1.73	0.54
17:AY:34:P5P:H8	17:AY:34:P5P:O5'	2.08	0.54
26:Ah:309:ASN:O	29:Ak:166:ARG:NH1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Ak:315:LYS:O	29:Ak:319:LYS:HB2	2.08	0.54
46:BA:615:A:OP1	46:BA:615:A:H2'	2.07	0.54
46:BA:661:C:C2	46:BA:778:G:N2	2.75	0.54
46:BA:790:G:H2'	46:BA:791:A:H8	1.72	0.54
57:BQ:117:ASN:HB3	57:BQ:166:ARG:HG3	1.90	0.54
60:BT:121:THR:HB	60:BT:131:SER:HB3	1.89	0.54
71:Bf:84:UNK:HA	71:Bf:92:UNK:CB	2.38	0.54
73:Bh:72:ILE:HD13	73:Bh:178:LEU:HD21	1.90	0.54
88:Bz:17:UNK:CA	88:Bz:20:UNK:HG3	2.37	0.54
1:AA:3:A:H3'	4:AE:335:LYS:HE3	1.90	0.54
1:AA:957:A:P	30:Am:24:ASN:HD21	2.31	0.54
6:AG:44:PRO:HD3	6:AG:75:LYS:HB2	1.89	0.54
6:AG:195:LYS:CB	6:AG:204:LYS:HZ2	2.18	0.54
34:As:2367:UNK:HA	34:As:2370:UNK:HG3	1.89	0.54
46:BA:99:C:H5	79:Bn:75:LYS:HZ1	1.55	0.54
50:BF:99:VAL:HG22	50:BF:165:LEU:HD23	1.89	0.54
50:BF:127:PRO:HD3	50:BF:139:GLY:O	2.08	0.54
56:BP:177:ALA:HA	56:BP:222:TYR:CD1	2.42	0.54
72:Bg:6:THR:HG22	72:Bg:7:ALA:H	1.73	0.54
78:Bm:74:HIS:ND1	78:Bm:77:GLU:OE2	2.40	0.54
2:AB:57:LEU:HB2	2:AB:270:TYR:CE2	2.40	0.54
7:AI:300:ASP:HB2	7:AI:303:LEU:HG	1.90	0.54
11:AN:91:CYS:SG	11:AN:94:THR:HG22	2.48	0.54
19:Aa:338:UNK:HA	19:Aa:341:UNK:HG3	1.89	0.54
23:Ae:243:UNK:HG1	23:Ae:245:UNK:HG3	1.83	0.54
23:Ae:399:UNK:C	23:Ae:402:UNK:HG3	2.38	0.54
28:Aj:160:THR:HB	28:Aj:161:PRO:HD2	1.90	0.54
32:Ao:189:UNK:HA	32:Ao:192:UNK:CG	2.38	0.54
32:Ao:267:UNK:HA	32:Ao:270:UNK:HG3	1.90	0.54
36:B0:76:HIS:HB2	36:B0:130:PHE:CE1	2.43	0.54
44:B8:124:ARG:NH2	46:BA:1202:A:OP1	2.41	0.54
46:BA:618:A:H5"	72:Bg:91:CYS:SG	2.47	0.54
46:BA:899:C:H3'	46:BA:923:G:C8	2.43	0.54
46:BA:1053:A:OP2	50:BF:134:GLY:HA2	2.08	0.54
46:BA:1238:A:O2'	46:BA:1239:U:O4'	2.26	0.54
56:BP:30:ASN:HD21	83:Bt:86:ARG:HH12	1.56	0.54
60:BT:268:ASP:HB3	60:BT:271:ARG:HB2	1.89	0.54
72:Bg:19:LEU:HD23	73:Bh:221:THR:HG22	1.88	0.54
75:Bj:51:LEU:HD13	75:Bj:192:LEU:HG	1.90	0.54
76:Bk:81:ASN:HB3	76:Bk:86:TYR:CZ	2.43	0.54
86:Bw:247:LEU:HD22	86:Bw:348:PRO:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:76:U:H4'	28:Aj:5:LYS:HE3	1.91	0.53
1:AA:177:U:H2'	1:AA:178:G:H8	1.73	0.53
1:AA:881:A:N3	23:Ae:66:UNK:CG	2.71	0.53
14:AQ:96:THR:HG23	22:Ad:120:ARG:NH1	2.23	0.53
20:Ab:62:ASP:OD1	20:Ab:62:ASP:N	2.32	0.53
21:Ac:114:GLU:HA	21:Ac:117:GLU:HG2	1.90	0.53
32:Ao:339:UNK:HG1	32:Ao:372:UNK:HB2	1.90	0.53
32:Ao:581:UNK:CG	32:Ao:654:UNK:CG	2.76	0.53
39:B3:148:ARG:HH21	39:B3:151:LEU:HD22	1.73	0.53
46:BA:721:A:H3'	46:BA:722:A:H5"	1.90	0.53
47:BB:11:Y5P:H4A	47:BB:12:Y5P:H4	1.88	0.53
49:BE:197:HIS:NE2	49:BE:318:THR:HG22	2.23	0.53
50:BF:49:ARG:NH1	50:BF:81:GLU:O	2.41	0.53
50:BF:116:THR:HG21	79:Bn:113:ARG:NH1	2.23	0.53
59:BS:149:THR:HG21	59:BS:151:TRP:CZ2	2.42	0.53
73:Bh:151:GLU:O	73:Bh:154:THR:HB	2.08	0.53
1:AA:270:C:OP1	33:Ap:80:ASN:ND2	2.42	0.53
1:AA:577:C:O3'	8:AJ:128:LYS:HD2	2.08	0.53
4:AE:124:LYS:HG3	4:AE:183:ARG:HH22	1.73	0.53
10:AL:61:VAL:HG23	10:AL:84:ARG:HB2	1.90	0.53
13:AP:36:ALA:HB2	13:AP:51:LEU:HD11	1.90	0.53
25:Ag:202:LYS:HZ3	25:Ag:220:PRO:HD3	1.73	0.53
32:Ao:514:UNK:CG	32:Ao:541:UNK:CG	2.63	0.53
46:BA:747:C:O2	64:BX:54:ARG:NH1	2.41	0.53
68:Bc:61:LYS:HD2	68:Bc:77:VAL:HG12	1.91	0.53
81:Bp:15:GLN:HE22	81:Bp:52:ILE:HD12	1.73	0.53
1:AA:180:U:H2'	1:AA:181:A:C8	2.43	0.53
4:AE:140:LEU:HD21	4:AE:160:ARG:HE	1.72	0.53
23:Ae:251:UNK:HA	23:Ae:254:UNK:HG3	1.91	0.53
26:Ah:301:LYS:HE2	32:Ao:139:CYS:HB2	1.91	0.53
32:Ao:475:UNK:HG2	32:Ao:506:UNK:HB2	1.90	0.53
38:B2:80:LYS:HZ3	74:Bi:71:ARG:NE	2.07	0.53
44:B8:113:ARG:HB3	56:BP:80:LYS:HA	1.91	0.53
46:BA:2:C:OP1	63:BW:48:LYS:N	2.39	0.53
46:BA:1017:C:H2'	46:BA:1018:C:H6	1.73	0.53
46:BA:1230:G:H8	46:BA:1230:G:H5"	1.73	0.53
46:BA:1509:A:P	87:Bx:160:LYS:HZ1	2.31	0.53
49:BE:49:TRP:CD1	49:BE:155:PHE:HB3	2.43	0.53
49:BE:317:PRO:HG2	49:BE:320:PHE:HE2	1.73	0.53
61:BU:52:LYS:HG2	61:BU:55:ARG:HH21	1.73	0.53
1:AA:714:U:H2'	1:AA:715:G:H8	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:163:VAL:HG21	3:AC:167:ILE:HD12	1.89	0.53
7:AI:87:HIS:CD2	29:Ak:84:PRO:HB2	2.43	0.53
17:AV:41:Y5P:H4A	17:AV:42:Y5P:C5	2.38	0.53
23:Ae:63:UNK:HG1	23:Ae:65:UNK:HG3	1.81	0.53
26:Ah:375:LYS:HD3	26:Ah:378:ILE:HD12	1.90	0.53
46:BA:195:U:O2'	46:BA:1012:A:OP1	2.25	0.53
46:BA:1139:A:H2'	46:BA:1140:U:C6	2.43	0.53
52:BJ:46:LYS:HE3	83:Bt:31:ALA:HB1	1.90	0.53
68:Bc:190:MET:HE3	68:Bc:291:ARG:HH11	1.73	0.53
69:Bd:102:PRO:HG2	69:Bd:103:PRO:HD3	1.91	0.53
80:Bo:97:GLU:O	80:Bo:101:GLU:HG2	2.09	0.53
84:Bu:101:ARG:NH1	84:Bu:131:GLU:HG3	2.23	0.53
1:AA:279:U:O2'	10:AL:54:GLY:O	2.26	0.53
1:AA:578:G:H3'	1:AA:579:A:H5"	1.91	0.53
17:AV:28:Y5P:N3	17:AV:29:Y5P:C5	2.71	0.53
17:AV:36:P5P:C6	17:AV:37:Y5P:H4	2.38	0.53
21:Ac:4:LYS:O	21:Ac:11:ARG:NH1	2.42	0.53
23:Ae:221:UNK:HA	23:Ae:224:UNK:CG	2.39	0.53
25:Ag:264:VAL:HG11	25:Ag:307:LEU:HD13	1.89	0.53
32:Ao:190:UNK:HG2	32:Ao:223:UNK:O	2.09	0.53
44:B8:113:ARG:HH11	56:BP:76:LEU:HA	1.72	0.53
48:BD:111:ARG:HH11	48:BD:111:ARG:HG3	1.73	0.53
49:BE:43:GLY:H	68:Bc:98:ARG:HH12	1.55	0.53
56:BP:88:SER:O	56:BP:134:ARG:HG3	2.09	0.53
62:BV:88:ASN:HD21	62:BV:208:LEU:H	1.56	0.53
67:Bb:308:GLN:C	80:Bo:113:LYS:HZ1	2.09	0.53
68:Bc:91:HIS:HB3	74:Bi:281:MET:HG3	1.91	0.53
86:Bw:182:LEU:HD11	86:Bw:416:VAL:HG22	1.91	0.53
88:Bz:304:UNK:O	88:Bz:307:UNK:HG3	2.09	0.53
1:AA:103:G:P	14:AQ:78:LYS:NZ	2.81	0.53
23:Ae:50:UNK:HG2	23:Ae:51:UNK:N	2.23	0.53
23:Ae:272:UNK:O	23:Ae:272:UNK:CG	2.57	0.53
25:Ag:338:PRO:HB3	29:Ak:294:TYR:HE2	1.73	0.53
32:Ao:492:UNK:O	32:Ao:496:UNK:HG3	2.08	0.53
37:B1:58:GLN:HG3	56:BP:89:PHE:CE1	2.44	0.53
37:B1:163:ARG:HD3	37:B1:205:GLY:H	1.73	0.53
46:BA:415:U:H2'	46:BA:416:G:C8	2.43	0.53
46:BA:677:U:H2'	46:BA:678:C:C6	2.44	0.53
46:BA:1129:U:O2'	51:BI:87:LYS:NZ	2.42	0.53
50:BF:283:LEU:HB2	56:BP:125:ARG:NH1	2.22	0.53
62:BV:60:LEU:HD13	87:Bx:185:VAL:HG12	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:Bv:142:ARG:C	85:Bv:145:UNK:HG3	2.34	0.53
1:AA:38:U:H4'	21:Ac:150:PRO:HB2	1.91	0.53
3:AC:98:GLY:HA3	27:Ai:71:TYR:CE1	2.43	0.53
4:AE:426:LYS:HG2	33:Ap:136:HIS:CE1	2.44	0.53
5:AF:3:ARG:HH11	5:AF:4:TYR:HE1	1.55	0.53
17:AY:55:Y5P:C6	17:AY:58:Y5P:C5	2.85	0.53
23:Ae:120:UNK:HG1	23:Ae:123:UNK:HG1	1.91	0.53
27:Ai:54:ASN:O	27:Ai:57:THR:OG1	2.26	0.53
29:Ak:196:VAL:HG12	29:Ak:199:ARG:HB2	1.91	0.53
33:Ap:89:ARG:HB2	33:Ap:144:MET:HE3	1.91	0.53
46:BA:160:A:H3'	46:BA:160:A:OP2	2.09	0.53
46:BA:366:A:C2	46:BA:432:G:C4	2.97	0.53
49:BE:316:PHE:CG	49:BE:316:PHE:O	2.62	0.53
50:BF:159:THR:OG1	79:Bn:90:ARG:NH1	2.41	0.53
54:BN:26:GLN:NE2	54:BN:147:GLN:OE1	2.42	0.53
58:BR:153:LEU:O	58:BR:157:GLN:HG2	2.09	0.53
60:BT:112:TYR:CE2	60:BT:215:VAL:HG11	2.44	0.53
64:BX:69:ARG:HH11	86:Bw:266:PRO:HD3	1.74	0.53
67:Bb:215:THR:HG23	67:Bb:237:VAL:O	2.08	0.53
74:Bi:240:ARG:NH1	74:Bi:274:GLN:HG3	2.24	0.53
79:Bn:35:ARG:HH12	79:Bn:39:PRO:HB3	1.73	0.53
1:AA:295:A:H1'	1:AA:487:C:H1'	1.90	0.53
1:AA:640:A:OP2	4:AE:242:ARG:NH1	2.42	0.53
32:Ao:416:UNK:O	32:Ao:420:UNK:HB1	2.09	0.53
46:BA:175:U:H2'	46:BA:176:U:C6	2.44	0.53
46:BA:801:A:O2'	46:BA:807:G:N7	2.33	0.53
46:BA:1189:A:H2'	46:BA:1190:U:H6	1.73	0.53
49:BE:67:ASP:HA	49:BE:70:LYS:HE3	1.91	0.53
52:BJ:36:HIS:O	52:BJ:37:ARG:HB3	2.09	0.53
56:BP:28:LYS:HZ2	56:BP:31:PRO:HD3	1.72	0.53
73:Bh:229:PHE:HB3	73:Bh:298:ARG:NH1	2.24	0.53
75:Bj:162:ARG:NH2	75:Bj:169:ASP:OD1	2.41	0.53
76:Bk:138:GLN:NE2	76:Bk:140:GLN:OE1	2.41	0.53
1:AA:344:G:H1	9:AK:121:ASN:CB	2.21	0.53
1:AA:505:U:H5	31:An:148:LYS:HG2	1.74	0.53
1:AA:647:A:H1'	2:AB:148:ARG:CZ	2.39	0.53
4:AE:149:MET:HG2	4:AE:154:VAL:H	1.74	0.53
6:AG:220:ILE:HG23	6:AG:223:LYS:HD3	1.90	0.53
10:AL:69:LYS:HZ2	10:AL:77:ASN:HB3	1.74	0.53
23:Ae:98:UNK:HG2	23:Ae:100:UNK:CG	2.39	0.53
23:Ae:392:UNK:O	23:Ae:395:UNK:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:Ao:579:UNK:O	32:Ao:582:UNK:HG3	2.09	0.53
37:B1:42:HIS:O	51:BI:55:ILE:HA	2.09	0.53
38:B2:166:ARG:NH2	38:B2:183:PHE:O	2.42	0.53
39:B3:142:ASN:ND2	39:B3:142:ASN:H	2.07	0.53
40:B4:63:SER:HA	69:Bd:179:THR:O	2.08	0.53
46:BA:96:U:H1'	46:BA:97:A:H5"	1.91	0.53
46:BA:1334:A:H2'	46:BA:1335:G:H8	1.74	0.53
50:BF:195:LEU:HD22	50:BF:196:PRO:HD2	1.90	0.53
52:BJ:173:PHE:HB3	81:Bp:51:VAL:HB	1.91	0.53
62:BV:139:LEU:HD12	62:BV:140:VAL:H	1.74	0.53
75:Bj:152:LYS:HB2	75:Bj:157:LEU:HD11	1.91	0.53
76:Bk:154:GLU:O	76:Bk:155:ARG:HD3	2.08	0.53
84:Bu:162:GLN:O	84:Bu:165:UNK:HG3	2.09	0.53
88:Bz:414:UNK:HA	88:Bz:417:UNK:HG3	1.90	0.53
1:AA:225:A:N6	1:AA:273:A:O5'	2.38	0.53
1:AA:529:G:H2'	1:AA:531:U:H5	1.73	0.53
4:AE:307:LYS:NZ	19:Aa:100:PRO:HG2	2.24	0.53
8:AJ:183:HIS:HE1	35:Az:708:UNK:CG	2.21	0.53
19:Aa:344:UNK:C	19:Aa:347:UNK:HG3	2.38	0.53
22:Ad:102:HIS:O	22:Ad:106:MET:HG2	2.08	0.53
28:Aj:171:ARG:HG3	28:Aj:189:PRO:HG3	1.91	0.53
31:An:144:ARG:NH1	31:An:147:VAL:HG11	2.22	0.53
46:BA:390:A:O2'	46:BA:391:U:O4'	2.27	0.53
46:BA:806:G:H2'	46:BA:807:G:H5"	1.91	0.53
48:BD:198:GLU:OE2	48:BD:203:ARG:N	2.42	0.53
50:BF:120:VAL:HG11	50:BF:142:ARG:HD2	1.91	0.53
52:BJ:37:ARG:HG3	52:BJ:37:ARG:O	2.09	0.53
54:BN:11:TRP:HE1	73:Bh:269:VAL:HG22	1.74	0.53
56:BP:11:ARG:HH11	56:BP:11:ARG:CG	2.15	0.53
56:BP:88:SER:OG	56:BP:134:ARG:NH2	2.41	0.53
61:BU:33:GLY:O	61:BU:36:ASN:ND2	2.42	0.53
73:Bh:68:TYR:O	73:Bh:72:ILE:HG12	2.08	0.53
78:Bm:126:ASP:OD1	78:Bm:126:ASP:N	2.39	0.53
1:AA:67:C:N3	22:Ad:27:ARG:HB2	2.24	0.52
23:Ae:67:UNK:C	23:Ae:100:UNK:HG1	2.39	0.52
23:Ae:177:UNK:O	23:Ae:181:UNK:HG3	2.09	0.52
23:Ae:376:UNK:O	23:Ae:380:UNK:HG2	2.09	0.52
23:Ae:406:UNK:C	23:Ae:407:UNK:HG3	2.39	0.52
25:Ag:296:VAL:HG11	25:Ag:307:LEU:HD11	1.91	0.52
25:Ag:333:PHE:HD2	29:Ak:302:LYS:HE2	1.73	0.52
37:B1:116:SER:OG	37:B1:142:ASP:OD1	2.21	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:B2:156:ARG:HA	70:Be:128:LEU:HD13	1.91	0.52
46:BA:175:U:H2'	46:BA:176:U:H6	1.74	0.52
56:BP:191:VAL:HB	56:BP:192:PRO:HD3	1.89	0.52
62:BV:90:LEU:HD11	71:Bf:61:TYR:HE1	1.74	0.52
66:Ba:393:LYS:HE3	66:Ba:394:LYS:HE3	1.90	0.52
71:Bf:79:UNK:O	71:Bf:79:UNK:HG2	2.08	0.52
79:Bn:69:HIS:CD2	79:Bn:71:LYS:H	2.17	0.52
86:Bw:374:THR:HG22	86:Bw:376:GLN:HB2	1.89	0.52
87:Bx:70:CYS:SG	87:Bx:108:CYS:HB3	2.49	0.52
11:AN:103:ARG:HB3	11:AN:104:TRP:CE3	2.44	0.52
19:Aa:340:UNK:O	19:Aa:344:UNK:HG2	2.09	0.52
23:Ae:51:UNK:HA	23:Ae:54:UNK:HG3	1.92	0.52
23:Ae:70:UNK:HG2	23:Ae:71:UNK:N	2.25	0.52
23:Ae:131:UNK:HG2	23:Ae:136:UNK:O	2.08	0.52
32:Ao:193:UNK:HA	32:Ao:196:UNK:HG3	1.91	0.52
32:Ao:343:UNK:O	32:Ao:347:UNK:HG3	2.10	0.52
32:Ao:480:UNK:HB1	32:Ao:513:UNK:HB1	1.90	0.52
32:Ao:511:UNK:HA	32:Ao:514:UNK:HG3	1.91	0.52
35:Az:705:UNK:CG	35:Az:706:UNK:N	2.72	0.52
38:B2:89:CYS:O	38:B2:93:ARG:HG2	2.09	0.52
44:B8:113:ARG:NH1	56:BP:76:LEU:HD23	2.23	0.52
49:BE:199:ARG:HH11	49:BE:199:ARG:HG3	1.73	0.52
64:BX:28:LEU:HD11	64:BX:40:VAL:CG1	2.40	0.52
65:BY:49:ILE:HD11	65:BY:117:HIS:CE1	2.44	0.52
71:Bf:83:UNK:O	71:Bf:95:UNK:HG1	2.09	0.52
1:AA:94:G:H4'	22:Ad:79:ARG:HH12	1.74	0.52
8:AJ:85:LYS:HG3	8:AJ:139:LEU:HD13	1.90	0.52
17:AV:54:Y5P:H4A	17:AV:55:Y5P:C4	2.37	0.52
19:Aa:134:ARG:CZ	19:Aa:185:TRP:HB3	2.39	0.52
23:Ae:68:UNK:HG2	23:Ae:71:UNK:HG3	1.89	0.52
23:Ae:294:UNK:O	23:Ae:297:UNK:HG3	2.09	0.52
25:Ag:160:TRP:CE3	25:Ag:288:LEU:HB3	2.44	0.52
32:Ao:512:UNK:HG2	32:Ao:513:UNK:N	2.24	0.52
33:Ap:73:VAL:O	33:Ap:74:TRP:CG	2.62	0.52
54:BN:135:GLU:HA	54:BN:138:LEU:HB2	1.92	0.52
56:BP:153:ASN:HB2	56:BP:256:LEU:HD23	1.90	0.52
74:Bi:288:LYS:HE3	74:Bi:291:GLU:HB2	1.90	0.52
75:Bj:235:LYS:NZ	76:Bk:172:GLU:HG2	2.24	0.52
79:Bn:46:ARG:HA	79:Bn:51:ARG:HD2	1.91	0.52
86:Bw:278:ILE:HB	86:Bw:336:TYR:CE2	2.44	0.52
7:AI:266:UNK:HG2	7:AI:268:MET:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AI:357:VAL:HG22	7:AI:361:GLU:OE1	2.09	0.52
11:AN:81:ASP:OD1	11:AN:81:ASP:N	2.42	0.52
21:Ac:24:LYS:HZ3	21:Ac:106:LEU:HA	1.73	0.52
23:Ae:127:UNK:O	23:Ae:131:UNK:CG	2.54	0.52
27:Ai:61:LEU:O	27:Ai:64:THR:OG1	2.28	0.52
32:Ao:116:ALA:O	32:Ao:120:ILE:HG12	2.09	0.52
39:B3:99:VAL:HG12	80:Bo:76:ARG:HE	1.74	0.52
46:BA:119:A:H5'	46:BA:120:C:OP2	2.09	0.52
49:BE:195:ALA:H	49:BE:281:ASN:HD22	1.57	0.52
63:BW:53:ASN:ND2	63:BW:72:TYR:O	2.41	0.52
67:Bb:158:TYR:O	67:Bb:163:HIS:N	2.42	0.52
75:Bj:191:THR:O	75:Bj:195:LEU:HB2	2.09	0.52
75:Bj:273:ARG:HA	75:Bj:276:LEU:HB3	1.91	0.52
88:Bz:9:UNK:C	88:Bz:12:UNK:HG3	2.40	0.52
3:AC:72:HIS:HB3	3:AC:112:ARG:NH1	2.24	0.52
3:AC:72:HIS:HB3	3:AC:112:ARG:HH11	1.73	0.52
4:AE:380:LEU:HD12	4:AE:381:PRO:HD2	1.91	0.52
8:AJ:119:THR:OG1	8:AJ:133:GLN:NE2	2.42	0.52
14:AQ:63:ILE:HB	14:AQ:86:PHE:HB2	1.90	0.52
17:AV:11:Y5P:H6	17:AV:11:Y5P:O5'	2.10	0.52
23:Ae:267:UNK:O	23:Ae:270:UNK:HG3	2.09	0.52
36:B0:51:PHE:HE2	36:B0:71:ARG:NH1	2.06	0.52
46:BA:528:A:H5'	46:BA:529:G:OP1	2.10	0.52
56:BP:248:THR:HA	56:BP:253:PHE:CD1	2.45	0.52
57:BQ:55:ARG:HA	57:BQ:99:TRP:CD1	2.44	0.52
59:BS:43:ALA:HB3	67:Bb:226:LEU:HD11	1.92	0.52
66:Ba:228:ALA:HB3	66:Ba:292:TYR:HB2	1.92	0.52
67:Bb:52:ARG:HD2	67:Bb:52:ARG:H	1.75	0.52
84:Bu:56:ASP:OD1	84:Bu:56:ASP:N	2.35	0.52
85:Bv:79:GLN:O	85:Bv:83:ARG:HG3	2.09	0.52
88:Bz:417:UNK:C	88:Bz:420:UNK:HG3	2.39	0.52
4:AE:206:PRO:HG2	4:AE:215:TYR:HD2	1.73	0.52
23:Ae:395:UNK:O	23:Ae:399:UNK:HG3	2.08	0.52
25:Ag:180:PRO:HB2	25:Ag:232:VAL:HG12	1.92	0.52
32:Ao:230:UNK:O	32:Ao:234:UNK:HG3	2.09	0.52
47:BB:43:Y5P:H2'	47:BB:44:Y5P:HA1	1.92	0.52
52:BJ:143:LEU:HD23	52:BJ:146:LEU:HD12	1.92	0.52
55:BO:125:SER:OG	55:BO:128:ARG:NH2	2.30	0.52
56:BP:285:PRO:HB3	56:BP:290:LEU:HD23	1.92	0.52
58:BR:139:ARG:HG3	58:BR:139:ARG:NH1	2.24	0.52
60:BT:60:UNK:O	60:BT:60:UNK:CG	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:Ba:350:ARG:NH1	66:Ba:384:GLN:O	2.43	0.52
83:Bt:9:ARG:HH11	83:Bt:9:ARG:CG	2.22	0.52
85:Bv:42:PRO:HA	85:Bv:52:LEU:HD11	1.92	0.52
4:AE:408:TRP:NE1	4:AE:412:LYS:HE2	2.25	0.52
8:AJ:151:SER:HB2	29:Ak:133:THR:HG22	1.92	0.52
17:AY:50:Y5P:H4A	17:AY:51:Y5P:H4	1.91	0.52
17:AY:74:Y5P:H4	46:BA:1376:U:C2	2.44	0.52
31:An:174:LYS:HE2	31:An:178:GLN:NE2	2.25	0.52
32:Ao:357:UNK:O	32:Ao:361:UNK:CG	2.52	0.52
32:Ao:498:UNK:O	32:Ao:502:UNK:HB1	2.10	0.52
32:Ao:539:UNK:HG1	32:Ao:583:UNK:HG1	1.87	0.52
41:B5:92:CYS:HG	46:BA:156:A:HO2'	1.57	0.52
46:BA:310:A:H5'	48:BD:262:GLY:HA2	1.92	0.52
46:BA:1379:A:H2'	46:BA:1380:C:O4'	2.09	0.52
58:BR:46:TRP:HD1	58:BR:122:ALA:HB2	1.74	0.52
65:BY:81:ARG:HH11	65:BY:81:ARG:HG2	1.74	0.52
66:Ba:144:ARG:HB3	66:Ba:194:LYS:NZ	2.24	0.52
66:Ba:221:GLN:HE21	66:Ba:223:HIS:HB2	1.75	0.52
68:Bc:71:ASP:OD2	68:Bc:96:TYR:OH	2.18	0.52
72:Bg:93:SER:O	72:Bg:97:ILE:HG12	2.10	0.52
77:Bl:80:PRO:HB2	77:Bl:82:LEU:HG	1.92	0.52
25:Ag:201:ILE:O	25:Ag:220:PRO:HA	2.09	0.52
28:Aj:121:LYS:HE3	28:Aj:123:LYS:HZ2	1.74	0.52
29:Ak:78:PHE:CE1	29:Ak:83:VAL:HG21	2.45	0.52
30:Am:95:GLU:HB3	30:Am:98:SER:HB3	1.92	0.52
32:Ao:158:UNK:O	32:Ao:161:UNK:HG3	2.09	0.52
35:Az:701:UNK:CG	35:Az:702:UNK:N	2.72	0.52
46:BA:172:C:H1'	71:Bf:126:ARG:HH12	1.75	0.52
46:BA:931:A:H1'	46:BA:1426:U:O2'	2.10	0.52
48:BD:136:ARG:HG2	48:BD:136:ARG:NH1	2.17	0.52
54:BN:25:MET:O	54:BN:149:ARG:NH1	2.43	0.52
61:BU:98:ASN:H	62:BV:109:GLN:NE2	2.07	0.52
67:Bb:261:ARG:NH2	84:Bu:124:ASN:HB3	2.24	0.52
69:Bd:146:ALA:HB2	75:Bj:211:GLY:HA2	1.91	0.52
83:Bt:24:PRO:CG	87:Bx:169:TRP:HB2	2.39	0.52
87:Bx:90:SER:HA	87:Bx:93:ILE:HD11	1.91	0.52
88:Bz:399:UNK:O	88:Bz:402:UNK:CG	2.57	0.52
1:AA:317:A:O2'	15:AR:103:LYS:N	2.43	0.52
4:AE:289:THR:HG23	4:AE:331:ASP:O	2.09	0.52
17:AY:55:Y5P:H5	17:AY:58:Y5P:H5	1.90	0.52
19:Aa:154:LYS:HZ3	19:Aa:181:ARG:CZ	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Ae:63:UNK:HG1	23:Ae:65:UNK:CG	2.39	0.52
23:Ae:109:UNK:HA	23:Ae:112:UNK:HG3	1.92	0.52
32:Ao:500:UNK:HA	32:Ao:503:UNK:HG3	1.90	0.52
38:B2:111:ARG:HG2	64:BX:25:PHE:CD1	2.45	0.52
55:BO:69:VAL:HG23	55:BO:89:HIS:ND1	2.24	0.52
62:BV:129:GLY:H	62:BV:164:VAL:HG13	1.73	0.52
63:BW:132:VAL:HG12	63:BW:133:GLU:O	2.10	0.52
64:BX:56:TYR:O	64:BX:60:ILE:HG12	2.10	0.52
65:BY:98:VAL:HG21	65:BY:109:ILE:HD12	1.92	0.52
67:Bb:293:LEU:HD21	67:Bb:335:LEU:HD13	1.91	0.52
1:AA:649:U:H3'	1:AA:650:A:H5"	1.92	0.52
3:AC:62:ILE:HA	3:AC:66:LYS:HB3	1.92	0.52
17:AY:3:Y5P:H6	17:AY:3:Y5P:O5'	2.10	0.52
19:Aa:198:ARG:NH2	33:Ap:171:GLU:O	2.43	0.52
21:Ac:94:SER:HB2	21:Ac:97:GLU:HG3	1.91	0.52
23:Ae:28:UNK:O	23:Ae:31:UNK:HG3	2.10	0.52
28:Aj:175:LEU:HA	28:Aj:178:ARG:HD3	1.91	0.52
32:Ao:197:UNK:HB2	32:Ao:203:UNK:HB2	1.91	0.52
32:Ao:486:UNK:O	32:Ao:486:UNK:HG3	2.10	0.52
46:BA:110:A:C4	46:BA:111:G:C8	2.97	0.52
46:BA:146:U:H1'	79:Bn:36:VAL:HG11	1.93	0.52
46:BA:467:A:H5"	46:BA:468:C:H5	1.74	0.52
46:BA:486:U:H3'	46:BA:487:C:O4'	2.09	0.52
46:BA:654:C:H1'	46:BA:655:U:C2	2.45	0.52
46:BA:720:A:H5'	66:Ba:300:ARG:HB2	1.91	0.52
46:BA:1240:U:O2'	46:BA:1241:U:OP2	2.28	0.52
48:BD:159:LYS:O	48:BD:162:ASP:HB2	2.10	0.52
61:BU:54:THR:HG21	62:BV:176:MET:N	2.11	0.52
63:BW:69:ALA:HB3	63:BW:178:GLU:HB3	1.92	0.52
68:Bc:48:GLU:O	68:Bc:52:GLN:HG2	2.10	0.52
69:Bd:157:LEU:HD21	75:Bj:178:TRP:CH2	2.45	0.52
72:Bg:59:PRO:HB2	73:Bh:77:HIS:HB3	1.91	0.52
81:Bp:74:LEU:HD13	81:Bp:93:HIS:CD2	2.45	0.52
1:AA:29:A:H2'	1:AA:30:A:C8	2.45	0.51
1:AA:954:U:H4'	1:AA:955:G:H5'	1.91	0.51
8:AJ:118:PHE:CD2	11:AN:101:LYS:NZ	2.79	0.51
20:Ab:101:GLU:O	20:Ab:105:GLU:HG2	2.10	0.51
33:Ap:179:THR:HG22	33:Ap:184:VAL:HG11	1.90	0.51
46:BA:747:C:H2'	70:Be:50:GLN:HE22	1.74	0.51
46:BA:1210:U:H5'	46:BA:1211:A:OP2	2.09	0.51
50:BF:97:HIS:HB2	56:BP:27:LEU:HD22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:BI:59:TRP:NE1	51:BI:81:LYS:HB3	2.23	0.51
54:BN:17:VAL:HG13	54:BN:142:VAL:HG21	1.92	0.51
60:BT:75:PHE:CD2	60:BT:110:GLU:HG3	2.44	0.51
70:Be:107:PHE:CE2	70:Be:109:PRO:HG3	2.45	0.51
71:Bf:92:UNK:C	71:Bf:95:UNK:HG3	2.27	0.51
83:Bt:11:ARG:HG2	83:Bt:12:ILE:N	2.24	0.51
84:Bu:81:CYS:HB2	84:Bu:97:LYS:HB3	1.92	0.51
84:Bu:166:UNK:C	84:Bu:167:UNK:HG3	2.39	0.51
1:AA:732:U:OP2	7:AI:306:PRO:HG2	2.10	0.51
1:AA:828:U:H2'	1:AA:829:G:H8	1.75	0.51
1:AA:828:U:H2'	1:AA:829:G:C8	2.46	0.51
8:AJ:136:MET:HE3	11:AN:123:VAL:HG13	1.92	0.51
13:AP:107:ALA:O	13:AP:111:ARG:HG3	2.08	0.51
21:Ac:129:PHE:CZ	21:Ac:137:ARG:HG3	2.45	0.51
25:Ag:201:ILE:HG12	25:Ag:255:PHE:HE1	1.75	0.51
25:Ag:265:ASN:HD21	25:Ag:310:SER:H	1.58	0.51
26:Ah:296:TRP:CZ3	26:Ah:301:LYS:HD2	2.45	0.51
32:Ao:363:UNK:HA	32:Ao:400:UNK:HB2	1.92	0.51
32:Ao:367:UNK:CG	32:Ao:368:UNK:N	2.73	0.51
36:B0:61:VAL:HG21	36:B0:97:VAL:HG23	1.91	0.51
38:B2:101:HIS:NE2	70:Be:61:PRO:HD3	2.24	0.51
63:BW:142:GLU:O	63:BW:174:VAL:HA	2.11	0.51
67:Bb:79:GLY:C	67:Bb:81:GLU:H	2.19	0.51
68:Bc:33:SER:HB2	68:Bc:36:GLU:HG3	1.91	0.51
71:Bf:83:UNK:HB2	71:Bf:95:UNK:HG2	1.93	0.51
82:Bq:106:LYS:HG3	82:Bq:108:GLU:H	1.75	0.51
1:AA:589:C:H2'	1:AA:590:C:C6	2.45	0.51
1:AA:856:U:H2'	1:AA:857:C:C6	2.45	0.51
21:Ac:19:GLY:HA3	21:Ac:54:GLN:CD	2.35	0.51
21:Ac:138:GLU:N	21:Ac:142:GLU:OE2	2.37	0.51
23:Ae:220:UNK:HA	23:Ae:223:UNK:CG	2.39	0.51
25:Ag:143:PHE:O	25:Ag:147:GLN:HG2	2.10	0.51
26:Ah:296:TRP:HZ3	26:Ah:301:LYS:HD2	1.75	0.51
32:Ao:287:UNK:HA	32:Ao:290:UNK:HG3	1.92	0.51
38:B2:80:LYS:HZ3	74:Bi:71:ARG:HH21	1.58	0.51
46:BA:319:U:O3'	48:BD:90:GLN:NE2	2.43	0.51
46:BA:718:C:OP2	48:BD:149:LYS:NZ	2.30	0.51
48:BD:170:ILE:HA	48:BD:187:ALA:HB2	1.93	0.51
49:BE:205:ASP:CG	49:BE:302:SER:HA	2.35	0.51
51:BI:122:ARG:O	51:BI:126:GLN:NE2	2.42	0.51
55:BO:74:LEU:HD12	55:BO:82:LYS:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:BO:128:ARG:HA	55:BO:138:LEU:HD21	1.91	0.51
66:Ba:201:ARG:HB3	66:Ba:230:LEU:HD11	1.90	0.51
72:Bg:117:LYS:HB2	72:Bg:119:PHE:CE1	2.45	0.51
81:Bp:16:VAL:HG22	81:Bp:66:VAL:HG13	1.91	0.51
86:Bw:278:ILE:O	86:Bw:329:TRP:HZ3	1.93	0.51
7:AI:85:LYS:HE2	7:AI:99:PHE:HB3	1.92	0.51
32:Ao:191:UNK:CA	32:Ao:194:UNK:HG3	2.38	0.51
32:Ao:224:UNK:HA	32:Ao:227:UNK:HG3	1.91	0.51
41:B5:156:THR:HG22	41:B5:173:ARG:HB3	1.93	0.51
43:B7:85:ARG:HH12	43:B7:90:ARG:HD2	1.76	0.51
55:BO:110:ASP:OD1	55:BO:110:ASP:N	2.36	0.51
63:BW:150:TYR:CE2	63:BW:168:VAL:HG13	2.46	0.51
68:Bc:177:CYS:HA	68:Bc:293:PHE:O	2.09	0.51
72:Bg:26:LEU:HD21	72:Bg:29:LEU:HD11	1.91	0.51
83:Bt:15:ARG:HG2	83:Bt:18:ILE:HD12	1.92	0.51
88:Bz:606:UNK:CA	88:Bz:609:UNK:HG3	2.39	0.51
1:AA:135:U:OP2	14:AQ:27:LYS:NZ	2.40	0.51
2:AB:70:ASP:O	2:AB:73:ASN:N	2.35	0.51
2:AB:71:PHE:CE2	2:AB:262:LYS:HG2	2.44	0.51
4:AE:314:LEU:H	4:AE:331:ASP:HA	1.75	0.51
17:AV:10:Y5P:O2'	88:Bz:425:UNK:CG	2.51	0.51
23:Ae:286:UNK:HA	23:Ae:289:UNK:HG3	1.91	0.51
32:Ao:359:UNK:HA	32:Ao:362:UNK:HG3	1.92	0.51
32:Ao:434:UNK:O	32:Ao:437:UNK:HG3	2.10	0.51
32:Ao:654:UNK:HA	32:Ao:657:UNK:HG3	1.92	0.51
41:B5:94:ARG:NH1	46:BA:642:G:OP2	2.43	0.51
46:BA:160:A:N6	46:BA:1034:A:H62	2.09	0.51
46:BA:198:A:H2'	46:BA:199:A:C8	2.46	0.51
46:BA:1529:C:H3'	46:BA:1530:U:H5"	1.92	0.51
49:BE:97:VAL:O	49:BE:197:HIS:HE1	1.94	0.51
52:BJ:111:LEU:O	52:BJ:115:GLN:HG2	2.10	0.51
56:BP:264:GLN:NE2	56:BP:269:LEU:O	2.23	0.51
61:BU:73:THR:HG23	61:BU:83:TYR:HB2	1.92	0.51
66:Ba:153:ARG:HD3	66:Ba:187:LEU:HD22	1.92	0.51
4:AE:225:VAL:HA	4:AE:243:VAL:HG12	1.92	0.51
17:AY:11:Y5P:H2'	17:AY:12:Y5P:H6	1.93	0.51
17:AY:25:Y5P:H2'	17:AY:26:Y5P:H6	1.91	0.51
17:AY:42:Y5P:HB	17:AY:43:Y5P:HB2	1.92	0.51
32:Ao:228:UNK:HB2	32:Ao:244:UNK:CG	2.40	0.51
32:Ao:240:UNK:C	32:Ao:243:UNK:HG3	2.41	0.51
32:Ao:264:UNK:HB2	32:Ao:289:UNK:CG	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:B3:73:LYS:NZ	46:BA:470:U:OP1	2.44	0.51
44:B8:138:ALA:HA	44:B8:141:LYS:HE3	1.93	0.51
46:BA:134:G:C6	65:BY:34:LYS:NZ	2.78	0.51
46:BA:503:U:H4'	46:BA:504:A:H5'	1.92	0.51
46:BA:658:C:H4'	58:BR:81:THR:CG2	2.39	0.51
49:BE:236:THR:O	49:BE:238:ARG:N	2.43	0.51
53:BK:23:ILE:HG12	53:BK:67:PRO:HB3	1.91	0.51
57:BQ:218:ILE:HG23	57:BQ:223:MET:HB2	1.93	0.51
75:Bj:276:LEU:HG	75:Bj:277:LEU:N	2.25	0.51
86:Bw:202:PHE:HE1	86:Bw:335:MET:HG3	1.76	0.51
88:Bz:35:UNK:HG2	88:Bz:36:UNK:N	2.24	0.51
7:AI:223:ILE:O	7:AI:227:GLU:HG2	2.11	0.51
19:Aa:311:UNK:O	19:Aa:315:UNK:CG	2.53	0.51
23:Ae:121:UNK:O	23:Ae:125:UNK:HG3	2.10	0.51
23:Ae:278:UNK:O	23:Ae:282:UNK:HG3	2.11	0.51
25:Ag:292:LEU:HD12	25:Ag:295:MET:HB3	1.93	0.51
33:Ap:107:ILE:HD11	33:Ap:150:LEU:HD11	1.93	0.51
39:B3:72:ILE:HD11	39:B3:118:ARG:HD3	1.93	0.51
44:B8:142:ARG:HH22	46:BA:1190:U:H5"	1.76	0.51
46:BA:55:A:H3'	46:BA:56:A:H4'	1.93	0.51
46:BA:219:G:H2'	46:BA:220:A:C8	2.46	0.51
46:BA:735:G:H1'	66:Ba:302:ARG:NH1	2.26	0.51
48:BD:186:GLY:HA3	48:BD:239:GLU:HG3	1.93	0.51
50:BF:69:LEU:O	50:BF:202:TYR:OH	2.27	0.51
63:BW:150:TYR:CD2	63:BW:168:VAL:HA	2.45	0.51
74:Bi:88:TYR:HD2	74:Bi:245:TYR:HE2	1.58	0.51
85:Bv:142:ARG:HA	85:Bv:145:UNK:CG	2.41	0.51
88:Bz:11:UNK:HA	88:Bz:14:UNK:HG3	1.91	0.51
7:AI:316:PHE:CD1	7:AI:370:LEU:HD21	2.46	0.51
12:AO:75:LEU:HD23	12:AO:106:LYS:HB3	1.92	0.51
17:AY:56:Y5P:O2'	17:AY:57:Y5P:O4'	2.29	0.51
23:Ae:280:UNK:C	23:Ae:283:UNK:HG3	2.40	0.51
32:Ao:88:VAL:O	32:Ao:110:LYS:NZ	2.44	0.51
32:Ao:185:UNK:O	32:Ao:188:UNK:HG3	2.10	0.51
45:B9:93:PRO:HB2	46:BA:1348:G:O3'	2.11	0.51
46:BA:624:G:O4'	50:BF:154:GLY:HA2	2.11	0.51
50:BF:49:ARG:HD2	50:BF:80:THR:HG23	1.92	0.51
67:Bb:212:SER:HB3	67:Bb:214:TRP:NE1	2.26	0.51
67:Bb:373:HIS:O	67:Bb:374:GLU:HG2	2.11	0.51
75:Bj:198:ASN:HB2	75:Bj:243:PHE:HA	1.92	0.51
84:Bu:108:ASP:OD1	84:Bu:108:ASP:N	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:Bv:97:ALA:O	85:Bv:101:GLU:HG2	2.11	0.51
3:AC:136:VAL:HG11	32:Ao:90:GLN:HE21	1.76	0.51
23:Ae:398:UNK:HA	23:Ae:401:UNK:CG	2.38	0.51
25:Ag:52:UNK:HG2	25:Ag:66:UNK:CG	2.18	0.51
25:Ag:330:LYS:O	25:Ag:334:ASP:HB2	2.11	0.51
30:Am:114:LYS:NZ	30:Am:116:HIS:HE1	2.08	0.51
32:Ao:225:UNK:CB	32:Ao:248:UNK:HG1	2.34	0.51
32:Ao:379:UNK:HA	32:Ao:382:UNK:HG3	1.92	0.51
37:B1:176:LEU:HD22	37:B1:188:TYR:CZ	2.46	0.51
43:B7:74:ARG:NH2	46:BA:32:C:OP2	2.44	0.51
46:BA:252:A:C2	46:BA:256:A:C6	2.99	0.51
54:BN:80:HIS:CD2	54:BN:82:GLY:H	2.29	0.51
57:BQ:232:PRO:O	57:BQ:235:LEU:HG	2.11	0.51
68:Bc:101:ILE:O	68:Bc:267:PRO:HD3	2.11	0.51
74:Bi:117:ALA:HB1	74:Bi:198:ARG:NH1	2.26	0.51
76:Bk:131:THR:CG2	88:Bz:101:UNK:HG3	2.41	0.51
1:AA:586:U:H5"	11:AN:90:ARG:HH21	1.76	0.51
1:AA:611:A:H2'	1:AA:612:U:O4'	2.11	0.51
1:AA:814:A:OP2	7:AI:378:ARG:NH1	2.43	0.51
8:AJ:102:LEU:HB3	8:AJ:104:ILE:HG13	1.93	0.51
9:AK:151:VAL:HG12	9:AK:177:ILE:HA	1.93	0.51
19:Aa:300:VAL:CG2	19:Aa:330:UNK:HG1	2.40	0.51
23:Ae:256:UNK:C	23:Ae:259:UNK:HG3	2.41	0.51
25:Ag:349:PRO:HG3	25:Ag:385:ARG:HH12	1.76	0.51
29:Ak:175:LEU:O	29:Ak:208:THR:HA	2.11	0.51
32:Ao:214:UNK:O	32:Ao:214:UNK:HG2	2.11	0.51
32:Ao:596:UNK:O	32:Ao:600:UNK:HB1	2.11	0.51
33:Ap:171:GLU:HB3	33:Ap:172:PRO:HD2	1.93	0.51
44:B8:140:ARG:HD2	46:BA:1204:U:OP1	2.11	0.51
46:BA:229:G:H2'	46:BA:230:C:C6	2.46	0.51
49:BE:202:GLN:NE2	49:BE:301:ASP:OD1	2.43	0.51
49:BE:285:VAL:HG12	49:BE:286:ASN:H	1.76	0.51
50:BF:211:ARG:HD2	78:Bm:59:ARG:CZ	2.40	0.51
57:BQ:72:ILE:HD11	57:BQ:96:TYR:CZ	2.45	0.51
76:Bk:126:ALA:HB2	76:Bk:155:ARG:NH1	2.27	0.51
1:AA:28:U:H2'	1:AA:29:A:C8	2.47	0.50
1:AA:648:A:OP1	2:AB:146:ARG:NH2	2.43	0.50
6:AG:116:GLU:OE2	25:Ag:85:ARG:NH1	2.41	0.50
23:Ae:173:UNK:HA	23:Ae:177:UNK:CG	2.41	0.50
23:Ae:218:UNK:HA	23:Ae:221:UNK:HG3	1.93	0.50
23:Ae:246:UNK:C	23:Ae:247:UNK:HG3	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Ae:296:UNK:HA	23:Ae:299:UNK:CG	2.40	0.50
30:Am:5:SER:HB3	30:Am:9:ARG:NH2	2.27	0.50
30:Am:59:ASN:O	30:Am:60:GLU:HG2	2.11	0.50
41:B5:95:ARG:NH1	46:BA:156:A:H5'	2.26	0.50
49:BE:129:VAL:HG23	49:BE:189:PRO:HA	1.92	0.50
62:BV:180:LYS:HD3	62:BV:181:ARG:HH12	1.76	0.50
68:Bc:91:HIS:ND1	74:Bi:281:MET:HB2	2.26	0.50
71:Bf:89:UNK:O	71:Bf:89:UNK:HG3	2.09	0.50
73:Bh:98:ILE:HD11	73:Bh:119:LEU:HB2	1.92	0.50
4:AE:374:ARG:NH1	19:Aa:100:PRO:HD3	2.27	0.50
7:AI:249:ILE:O	7:AI:249:ILE:HG13	2.11	0.50
8:AJ:158:GLU:HG2	32:Ao:70:ILE:HG21	1.94	0.50
23:Ae:359:UNK:HA	23:Ae:362:UNK:HG3	1.92	0.50
24:Af:144:ARG:HB2	24:Af:171:LEU:HD11	1.94	0.50
36:B0:102:GLU:HB2	36:B0:130:PHE:CE2	2.47	0.50
46:BA:163:A:OP1	61:BU:52:LYS:NZ	2.43	0.50
49:BE:206:VAL:HG11	49:BE:289:VAL:HG13	1.92	0.50
50:BF:276:HIS:HA	50:BF:279:ARG:HG2	1.92	0.50
53:BK:140:VAL:O	53:BK:144:ILE:HG12	2.12	0.50
56:BP:233:ARG:HH21	56:BP:247:ILE:HG12	1.76	0.50
67:Bb:374:GLU:HB2	84:Bu:140:ARG:NH2	2.27	0.50
72:Bg:41:ARG:HA	72:Bg:44:ARG:HH21	1.76	0.50
88:Bz:311:UNK:C	88:Bz:314:UNK:HG3	2.40	0.50
8:AJ:72:LEU:HG	29:Ak:135:TRP:CZ3	2.46	0.50
13:AP:117:GLU:HA	13:AP:120:LEU:HB2	1.93	0.50
17:AY:70:Y5P:C4	17:AY:71:Y5P:H4	2.29	0.50
23:Ae:73:UNK:HG2	23:Ae:74:UNK:N	2.25	0.50
23:Ae:75:UNK:HA	23:Ae:78:UNK:HG3	1.92	0.50
23:Ae:309:UNK:HG2	23:Ae:309:UNK:O	2.09	0.50
32:Ao:192:UNK:C	32:Ao:195:UNK:HG3	2.41	0.50
41:B5:91:ARG:NH2	46:BA:153:A:OP2	2.44	0.50
46:BA:350:A:H3'	46:BA:352:C:N4	2.26	0.50
46:BA:353:U:H2'	46:BA:354:G:H8	1.74	0.50
46:BA:562:A:N3	46:BA:1337:A:O2'	2.36	0.50
46:BA:1011:A:H2'	46:BA:1012:A:O4'	2.11	0.50
46:BA:1351:C:OP2	46:BA:1356:G:N2	2.44	0.50
46:BA:1547:A:H2	71:Bf:104:GLU:HG2	1.76	0.50
49:BE:164:PHE:HD1	49:BE:165:TYR:CD1	2.30	0.50
56:BP:248:THR:HA	56:BP:253:PHE:CE1	2.47	0.50
62:BV:168:THR:HG23	62:BV:194:GLN:HB2	1.93	0.50
63:BW:130:HIS:CE1	74:Bi:227:ARG:NH1	2.79	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:Bb:87:ARG:HD2	67:Bb:166:THR:OG1	2.12	0.50
67:Bb:261:ARG:NH1	67:Bb:341:VAL:HG21	2.26	0.50
75:Bj:64:THR:HG22	75:Bj:66:LEU:H	1.75	0.50
1:AA:102:G:H5'	14:AQ:75:LYS:HZ2	1.75	0.50
7:AI:94:GLU:HB2	7:AI:99:PHE:HE2	1.76	0.50
7:AI:197:GLY:O	7:AI:249:ILE:HG12	2.11	0.50
17:AV:42:Y5P:H4A	17:AV:43:Y5P:C4	2.37	0.50
20:Ab:65:TYR:HB2	20:Ab:67:GLU:HG3	1.93	0.50
32:Ao:322:UNK:HA	32:Ao:325:UNK:HG3	1.93	0.50
37:B1:115:TYR:HD1	37:B1:122:ARG:HG2	1.76	0.50
46:BA:1018:C:H2'	46:BA:1019:C:C6	2.46	0.50
46:BA:1141:U:H2'	46:BA:1142:U:C6	2.45	0.50
46:BA:1403:A:H2'	46:BA:1404:G:O4'	2.11	0.50
47:BB:36:P5P:H2'	47:BB:37:P5P:O4'	2.10	0.50
48:BD:111:ARG:NE	48:BD:152:ILE:HD12	2.26	0.50
53:BK:97:ILE:HD11	53:BK:153:ILE:HD11	1.93	0.50
56:BP:141:VAL:HG12	56:BP:142:GLU:H	1.77	0.50
76:Bk:86:TYR:HE1	76:Bk:88:TYR:HD1	1.59	0.50
88:Bz:406:UNK:HA	88:Bz:409:UNK:HG3	1.94	0.50
1:AA:671:U:H2'	1:AA:672:A:C8	2.46	0.50
2:AB:58:ARG:O	2:AB:61:ILE:HG22	2.10	0.50
5:AF:22:LEU:HD22	5:AF:39:LEU:HD11	1.93	0.50
23:Ae:92:UNK:HG3	23:Ae:93:UNK:N	2.27	0.50
23:Ae:120:UNK:HB2	23:Ae:123:UNK:HG3	1.94	0.50
32:Ao:224:UNK:O	32:Ao:227:UNK:HG3	2.12	0.50
32:Ao:240:UNK:O	32:Ao:243:UNK:HG3	2.11	0.50
33:Ap:189:PRO:HB3	33:Ap:193:LEU:HD12	1.93	0.50
39:B3:79:PRO:HD2	39:B3:82:GLU:HG3	1.93	0.50
46:BA:41:A:H2'	46:BA:42:C:H4'	1.94	0.50
46:BA:602:A:H2'	46:BA:603:C:O4'	2.12	0.50
49:BE:212:GLY:O	58:BR:11:HIS:HE1	1.95	0.50
64:BX:66:ALA:HB2	64:BX:100:ALA:HA	1.93	0.50
68:Bc:153:ARG:HH12	68:Bc:256:ASP:HB2	1.76	0.50
75:Bj:53:LEU:HD11	75:Bj:238:LEU:HD21	1.93	0.50
1:AA:744:C:O2'	1:AA:746:A:O2'	2.24	0.50
2:AB:161:CYS:SG	2:AB:253:GLN:HA	2.51	0.50
8:AJ:170:MET:HE3	8:AJ:172:VAL:HG23	1.93	0.50
16:AU:70:ARG:HG2	24:Af:154:PHE:HE1	1.76	0.50
17:AV:37:Y5P:C5	17:AV:38:Y5P:C5	2.89	0.50
23:Ae:221:UNK:CG	23:Ae:253:UNK:HB1	2.42	0.50
29:Ak:189:LYS:HE2	29:Ak:193:ILE:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Ak:199:ARG:HG2	29:Ak:199:ARG:HH11	1.76	0.50
32:Ao:375:UNK:HA	32:Ao:378:UNK:HG3	1.94	0.50
35:Az:700:UNK:O	35:Az:704:UNK:HG3	2.12	0.50
37:B1:79:LEU:HD21	37:B1:157:PHE:HD1	1.77	0.50
41:B5:165:PRO:HB3	41:B5:174:ILE:HD11	1.93	0.50
46:BA:858:G:O5'	48:BD:136:ARG:NH2	2.44	0.50
46:BA:1078:A:H61	46:BA:1134:U:H3	1.58	0.50
54:BN:4:PHE:CE2	73:Bh:285:PRO:HD3	2.47	0.50
56:BP:178:PHE:HB2	56:BP:214:TYR:CZ	2.46	0.50
68:Bc:138:ALA:HA	68:Bc:141:ARG:HD2	1.93	0.50
72:Bg:144:ARG:HH22	73:Bh:260:GLN:NE2	2.10	0.50
81:Bp:62:PRO:HG2	81:Bp:78:GLY:O	2.12	0.50
86:Bw:140:VAL:HG22	86:Bw:174:LEU:HD11	1.92	0.50
1:AA:124:A:H5'	1:AA:125:U:OP1	2.11	0.50
3:AC:124:LEU:HD11	3:AC:160:SER:HA	1.94	0.50
23:Ae:71:UNK:HA	23:Ae:74:UNK:CG	2.36	0.50
23:Ae:221:UNK:HG1	23:Ae:253:UNK:HB1	1.93	0.50
32:Ao:436:UNK:HA	32:Ao:439:UNK:HG3	1.94	0.50
46:BA:785:U:H2'	46:BA:786:A:O4'	2.12	0.50
46:BA:1417:C:H2'	46:BA:1418:A:O4'	2.12	0.50
49:BE:90:TRP:CH2	49:BE:92:PRO:HA	2.47	0.50
49:BE:221:ARG:NH1	49:BE:259:GLY:HA3	2.27	0.50
50:BF:61:PRO:HA	50:BF:84:PRO:HD3	1.93	0.50
54:BN:75:LYS:HB2	87:Bx:174:MET:HE1	1.94	0.50
55:BO:51:TYR:CE2	55:BO:78:ARG:HA	2.47	0.50
57:BQ:81:GLU:O	57:BQ:123:ARG:NH2	2.44	0.50
66:Ba:188:CYS:HB3	66:Ba:418:TYR:CD2	2.47	0.50
68:Bc:296:LEU:HD21	68:Bc:312:LEU:HB3	1.93	0.50
74:Bi:84:ILE:HG21	74:Bi:247:VAL:HG21	1.94	0.50
76:Bk:96:ILE:HG23	76:Bk:154:GLU:HG2	1.92	0.50
88:Bz:605:UNK:C	88:Bz:608:UNK:HG3	2.40	0.50
3:AC:73:THR:HG23	8:AJ:169:ALA:HB2	1.94	0.50
3:AC:93:ARG:HH11	3:AC:108:LEU:HB3	1.77	0.50
4:AE:362:LEU:HG	19:Aa:104:LEU:HD21	1.93	0.50
4:AE:370:VAL:HG22	4:AE:385:ALA:HB3	1.93	0.50
11:AN:60:ASN:HD22	11:AN:63:LEU:HG	1.76	0.50
17:AY:6:Y5P:O5'	17:AY:6:Y5P:H6	2.12	0.50
23:Ae:301:UNK:HA	23:Ae:304:UNK:CG	2.39	0.50
24:Af:156:GLY:HA3	30:Am:28:ILE:HD13	1.93	0.50
29:Ak:254:ILE:HG22	29:Ak:256:GLU:H	1.77	0.50
32:Ao:173:UNK:HA	32:Ao:176:UNK:HG3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:Ao:192:UNK:HA	32:Ao:195:UNK:HG3	1.93	0.50
32:Ao:400:UNK:HG3	32:Ao:401:UNK:N	2.26	0.50
32:Ao:503:UNK:HB2	32:Ao:513:UNK:CG	2.39	0.50
41:B5:125:TYR:O	41:B5:128:GLU:HB2	2.12	0.50
46:BA:434:C:H1'	46:BA:467:A:C8	2.46	0.50
46:BA:529:G:HO2'	82:Bq:127:TRP:HE1	1.51	0.50
46:BA:1202:A:N7	67:Bb:360:ARG:NH2	2.59	0.50
46:BA:1209:A:P	59:BS:176:ARG:HH22	2.34	0.50
46:BA:1343:A:H2	46:BA:1364:A:H61	1.59	0.50
48:BD:69:ARG:HH11	48:BD:69:ARG:CB	2.24	0.50
51:BI:130:VAL:HB	51:BI:136:ASN:ND2	2.26	0.50
59:BS:89:HIS:CG	59:BS:119:THR:HG21	2.46	0.50
64:BX:71:ARG:NH1	64:BX:71:ARG:HG2	2.27	0.50
65:BY:122:LEU:HD23	65:BY:133:VAL:HG21	1.94	0.50
68:Bc:229:HIS:CD2	68:Bc:229:HIS:H	2.29	0.50
72:Bg:28:ARG:HB3	72:Bg:28:ARG:HH11	1.77	0.50
74:Bi:254:ASP:OD2	74:Bi:257:GLY:N	2.45	0.50
1:AA:939:A:H2'	1:AA:940:C:H6	1.77	0.50
7:AI:87:HIS:CE1	29:Ak:64:VAL:HA	2.47	0.50
7:AI:260:UNK:CG	7:AI:355:SER:HB3	2.39	0.50
9:AK:113:SER:O	9:AK:117:GLU:HB2	2.11	0.50
10:AL:81:CYS:HB2	10:AL:95:ILE:HD11	1.94	0.50
12:AO:196:TYR:HB3	12:AO:198:ARG:HD2	1.93	0.50
14:AQ:35:LEU:HB2	14:AQ:42:TYR:CZ	2.47	0.50
15:AR:65:LYS:HB3	15:AR:69:CYS:HB2	1.94	0.50
15:AR:114:ARG:O	15:AR:118:LEU:HG	2.11	0.50
23:Ae:58:UNK:O	23:Ae:62:UNK:CG	2.33	0.50
23:Ae:223:UNK:C	23:Ae:226:UNK:HG3	2.42	0.50
32:Ao:267:UNK:HA	32:Ao:270:UNK:CG	2.42	0.50
41:B5:127:TYR:OH	58:BR:43:GLU:OE1	2.29	0.50
46:BA:257:C:H2'	46:BA:258:C:O4'	2.11	0.50
46:BA:732:A:OP2	48:BD:105:ARG:NH2	2.45	0.50
48:BD:69:ARG:HB2	48:BD:69:ARG:NH1	2.25	0.50
48:BD:128:ILE:HD11	48:BD:144:ALA:HB3	1.93	0.50
66:Ba:108:HIS:CD2	66:Ba:110:ARG:H	2.21	0.50
68:Bc:93:SER:OG	68:Bc:95:TRP:HB2	2.12	0.50
1:AA:368:A:P	9:AK:186:ASN:HD22	2.35	0.49
1:AA:836:G:H2'	1:AA:837:C:C6	2.47	0.49
3:AC:75:ASN:HD21	11:AN:104:TRP:HE1	1.60	0.49
3:AC:89:ASP:CG	3:AC:110:LEU:HD12	2.37	0.49
17:AY:2:Y5P:H4A	17:AY:3:Y5P:H4	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Aa:78:LEU:HD21	19:Aa:271:ALA:HB3	1.94	0.49
23:Ae:124:UNK:HA	23:Ae:127:UNK:CG	2.42	0.49
23:Ae:302:UNK:O	23:Ae:305:UNK:HG3	2.12	0.49
37:B1:41:VAL:HG11	37:B1:83:GLU:HB3	1.93	0.49
39:B3:121:PRO:HG3	83:Bt:48:TRP:CH2	2.46	0.49
46:BA:134:G:H1	65:BY:34:LYS:HZ3	1.59	0.49
46:BA:437:A:O3'	57:BQ:231:SER:HB2	2.12	0.49
46:BA:687:A:N1	63:BW:155:ARG:HG3	2.27	0.49
46:BA:859:U:H2'	48:BD:209:ARG:HD2	1.95	0.49
46:BA:878:C:O2'	46:BA:920:A:N3	2.39	0.49
46:BA:983:C:H2'	46:BA:984:U:C6	2.47	0.49
46:BA:1024:A:C6	46:BA:1319:C:H1'	2.47	0.49
46:BA:1194:G:H8	46:BA:1194:G:O5'	1.95	0.49
46:BA:1395:G:H2'	46:BA:1396:U:O4'	2.12	0.49
46:BA:1483:A:H2'	46:BA:1484:A:C8	2.47	0.49
50:BF:175:LYS:NZ	50:BF:277:ASN:OD1	2.44	0.49
59:BS:61:VAL:HG13	67:Bb:346:ARG:HH22	1.76	0.49
59:BS:90:ILE:O	59:BS:107:THR:OG1	2.30	0.49
61:BU:65:ARG:NH1	61:BU:99:ARG:HH11	2.10	0.49
68:Bc:174:GLY:N	68:Bc:315:ARG:NH1	2.59	0.49
76:Bk:131:THR:HG22	88:Bz:101:UNK:HG3	1.94	0.49
78:Bm:58:SER:C	78:Bm:60:THR:H	2.20	0.49
79:Bn:119:LYS:O	79:Bn:123:ARG:HB2	2.11	0.49
88:Bz:605:UNK:O	88:Bz:608:UNK:CG	2.51	0.49
1:AA:194:U:H2'	1:AA:195:G:H8	1.75	0.49
1:AA:505:U:C5	31:An:148:LYS:HG2	2.47	0.49
17:AV:27:Y5P:H4A	17:AV:28:Y5P:H4	1.94	0.49
20:Ab:86:ASP:OD2	20:Ab:88:PHE:HB2	2.12	0.49
23:Ae:246:UNK:O	23:Ae:246:UNK:HG2	2.11	0.49
32:Ao:194:UNK:CB	32:Ao:230:UNK:HG1	2.42	0.49
40:B4:51:ARG:HB2	75:Bj:84:TYR:O	2.11	0.49
42:B6:41:LEU:HB3	42:B6:58:GLU:HB2	1.94	0.49
47:BB:13:Y5P:H4	47:BB:24:P5P:N1	2.26	0.49
52:BJ:128:ASN:ND2	52:BJ:147:PHE:O	2.43	0.49
54:BN:81:THR:OG1	54:BN:86:GLY:O	2.29	0.49
54:BN:94:GLN:O	54:BN:97:GLN:HB3	2.11	0.49
56:BP:260:LYS:HG3	56:BP:267:PHE:CE1	2.47	0.49
59:BS:149:THR:HG21	59:BS:151:TRP:CH2	2.47	0.49
65:BY:199:MET:HG3	65:BY:204:ILE:HB	1.93	0.49
66:Ba:361:THR:HG22	66:Ba:363:ASP:H	1.78	0.49
67:Bb:212:SER:HB3	67:Bb:214:TRP:HE1	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:Bj:159:LEU:HD11	75:Bj:252:HIS:HB2	1.95	0.49
88:Bz:601:UNK:HG2	88:Bz:602:UNK:N	2.26	0.49
1:AA:102:G:O3'	14:AQ:78:LYS:NZ	2.45	0.49
1:AA:551:G:H21	1:AA:778:G:H4'	1.77	0.49
1:AA:675:A:OP1	3:AC:41:ARG:NH1	2.46	0.49
1:AA:924:U:H4'	1:AA:945:A:H2	1.76	0.49
3:AC:42:VAL:HG13	3:AC:49:LYS:NZ	2.27	0.49
3:AC:84:GLU:HB2	3:AC:85:ARG:NH1	2.28	0.49
17:AV:27:Y5P:H2'	17:AV:28:Y5P:C6	2.43	0.49
23:Ae:247:UNK:O	23:Ae:247:UNK:CG	2.51	0.49
29:Ak:128:LEU:HD21	32:Ao:70:ILE:HG23	1.92	0.49
32:Ao:274:UNK:HG2	32:Ao:275:UNK:N	2.26	0.49
42:B6:34:ARG:NE	46:BA:1183:A:OP2	2.45	0.49
46:BA:206:A:OP1	79:Bn:86:ASN:ND2	2.45	0.49
46:BA:1007:A:H2'	46:BA:1008:A:C8	2.47	0.49
52:BJ:93:ASN:ND2	52:BJ:155:VAL:HG22	2.28	0.49
54:BN:139:LYS:O	72:Bg:144:ARG:NE	2.46	0.49
56:BP:246:ASP:HA	84:Bu:61:LEU:HD11	1.95	0.49
61:BU:24:VAL:HG12	61:BU:25:LEU:HD23	1.94	0.49
64:BX:15:PRO:HG3	65:BY:208:ARG:O	2.11	0.49
65:BY:92:ASN:O	65:BY:112:GLU:HA	2.13	0.49
67:Bb:197:GLU:OE1	67:Bb:197:GLU:N	2.45	0.49
73:Bh:92:PHE:CE1	73:Bh:178:LEU:HB3	2.47	0.49
77:Bl:88:ARG:HB3	77:Bl:92:HIS:HA	1.93	0.49
85:Bv:104:ARG:HA	85:Bv:107:GLN:HG2	1.93	0.49
1:AA:211:A:H2'	1:AA:212:A:O4'	2.12	0.49
1:AA:217:U:H2'	1:AA:218:A:C8	2.48	0.49
1:AA:320:A:H61	1:AA:390:A:H1'	1.76	0.49
1:AA:629:C:H2'	1:AA:630:A:C8	2.48	0.49
1:AA:807:G:O6	1:AA:809:G:N2	2.46	0.49
4:AE:160:ARG:HD2	4:AE:165:GLN:NE2	2.26	0.49
6:AG:57:GLU:HB2	6:AG:60:GLU:HB2	1.93	0.49
7:AI:94:GLU:HB2	7:AI:99:PHE:CE2	2.48	0.49
14:AQ:29:ARG:NH1	14:AQ:46:ARG:NH1	2.60	0.49
17:AV:35:P5P:H8	17:AV:35:P5P:O5'	2.13	0.49
17:AV:63:Y5P:H2'	17:AV:64:Y5P:H6	1.94	0.49
23:Ae:124:UNK:CA	23:Ae:127:UNK:HG3	2.42	0.49
23:Ae:166:UNK:O	23:Ae:171:UNK:HG3	2.11	0.49
24:Af:101:VAL:HG21	24:Af:145:LEU:HD13	1.94	0.49
25:Ag:161:VAL:HG21	25:Ag:266:ALA:HB1	1.93	0.49
32:Ao:655:UNK:HG2	32:Ao:674:UNK:CB	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:B3:71:ARG:HH12	39:B3:94:ALA:N	2.11	0.49
46:BA:138:G:O6	74:Bi:72:LEU:HB3	2.12	0.49
46:BA:786:A:C4	58:BR:17:ARG:HD2	2.47	0.49
47:BB:25:P5P:C6	47:BB:26:Y5P:H4	2.43	0.49
50:BF:97:HIS:CE1	56:BP:29:PRO:HD3	2.48	0.49
67:Bb:239:ASN:O	67:Bb:241:PRO:HD3	2.13	0.49
72:Bg:17:ASN:HD21	72:Bg:23:VAL:N	2.03	0.49
75:Bj:79:ILE:O	75:Bj:82:SER:OG	2.28	0.49
82:Bq:110:LEU:HD12	82:Bq:111:ASP:H	1.78	0.49
85:Bv:150:UNK:HA	85:Bv:153:UNK:HG3	1.93	0.49
87:Bx:144:LYS:H	87:Bx:144:LYS:HD2	1.76	0.49
1:AA:397:U:H2'	1:AA:398:G:O4'	2.13	0.49
1:AA:821:A:H5'	1:AA:822:A:OP2	2.12	0.49
1:AA:904:A:H2'	1:AA:905:U:C6	2.47	0.49
3:AC:106:ASP:HB3	29:Ak:105:LEU:HD22	1.94	0.49
7:AI:263:UNK:CG	7:AI:265:UNK:HG3	2.42	0.49
20:Ab:8:THR:HG23	20:Ab:46:PHE:CD2	2.48	0.49
23:Ae:296:UNK:C	23:Ae:299:UNK:HG3	2.43	0.49
26:Ah:292:GLU:HG3	26:Ah:296:TRP:CD1	2.47	0.49
29:Ak:290:GLU:OE1	29:Ak:320:ARG:HD3	2.13	0.49
37:B1:93:ASN:O	37:B1:94:ASN:HB2	2.13	0.49
37:B1:168:ARG:HH21	37:B1:175:GLN:HG3	1.78	0.49
46:BA:275:G:C5	48:BD:260:LYS:HB2	2.47	0.49
54:BN:8:PRO:HB2	73:Bh:285:PRO:HG2	1.93	0.49
60:BT:62:UNK:O	60:BT:62:UNK:HG2	2.12	0.49
67:Bb:333:GLN:HB3	67:Bb:334:LEU:HD23	1.94	0.49
86:Bw:132:ASP:O	86:Bw:136:LEU:HG	2.11	0.49
1:AA:519:A:C2	1:AA:520:G:H1'	2.47	0.49
4:AE:282:ILE:HG23	4:AE:353:LEU:HB3	1.93	0.49
8:AJ:117:ARG:HG2	8:AJ:135:GLU:HG3	1.95	0.49
19:Aa:220:GLN:HB2	19:Aa:222:GLN:HG3	1.94	0.49
19:Aa:322:UNK:CG	19:Aa:325:UNK:CG	2.91	0.49
23:Ae:93:UNK:C	23:Ae:96:UNK:HG3	2.42	0.49
25:Ag:221:LEU:HD12	25:Ag:224:VAL:HB	1.94	0.49
28:Aj:30:ASP:N	28:Aj:30:ASP:OD1	2.45	0.49
32:Ao:598:UNK:HG1	32:Ao:670:UNK:HB2	1.94	0.49
46:BA:356:U:H6	46:BA:356:U:H5"	1.76	0.49
46:BA:688:U:H1'	46:BA:1003:G:H21	1.78	0.49
46:BA:1197:A:H2'	46:BA:1198:A:O4'	2.12	0.49
52:BJ:89:VAL:HG22	52:BJ:124:LYS:HZ2	1.76	0.49
60:BT:59:UNK:O	60:BT:59:UNK:CG	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:BX:140:ARG:NH1	68:Bc:63:GLU:OE2	2.46	0.49
66:Ba:203:CYS:HB3	86:Bw:173:GLN:NE2	2.28	0.49
68:Bc:132:PRO:O	68:Bc:135:VAL:N	2.46	0.49
69:Bd:173:ARG:NH2	75:Bj:56:PRO:HB3	2.27	0.49
72:Bg:13:SER:OG	72:Bg:17:ASN:N	2.46	0.49
72:Bg:15:LEU:HD11	73:Bh:169:VAL:HA	1.95	0.49
73:Bh:59:ARG:HG2	73:Bh:184:PHE:HB2	1.94	0.49
73:Bh:240:LEU:O	73:Bh:244:GLU:HG2	2.13	0.49
1:AA:124:A:H4'	1:AA:125:U:O5'	2.12	0.49
1:AA:719:U:H2'	1:AA:720:A:O4'	2.12	0.49
1:AA:750:G:H2'	1:AA:751:A:H5"	1.94	0.49
1:AA:846:C:H2'	1:AA:847:C:O4'	2.13	0.49
4:AE:309:PRO:HB3	4:AE:374:ARG:HH12	1.78	0.49
9:AK:64:ILE:HG22	9:AK:66:PRO:HD2	1.94	0.49
16:AU:48:PRO:O	16:AU:52:ARG:HD3	2.12	0.49
17:AV:28:Y5P:C2	17:AV:29:Y5P:C5	2.90	0.49
25:Ag:173:ASN:HB3	25:Ag:176:ARG:HD2	1.94	0.49
27:Ai:46:LYS:O	27:Ai:50:ASP:HB2	2.13	0.49
33:Ap:187:THR:O	33:Ap:189:PRO:HD3	2.13	0.49
46:BA:462:A:H5"	46:BA:463:U:H5'	1.94	0.49
46:BA:560:A:H3'	46:BA:560:A:N3	2.28	0.49
46:BA:1556:U:C2	49:BE:292:HIS:CD2	3.01	0.49
47:BB:44:Y5P:H2'	47:BB:45:P5P:H8	1.95	0.49
48:BD:193:LEU:O	48:BD:246:GLY:N	2.45	0.49
49:BE:111:THR:HG22	49:BE:115:GLN:O	2.11	0.49
75:Bj:152:LYS:NZ	75:Bj:256:SER:OG	2.44	0.49
75:Bj:257:LYS:HD3	75:Bj:276:LEU:HD21	1.94	0.49
83:Bt:50:SER:O	83:Bt:52:PRO:HD3	2.12	0.49
88:Bz:401:UNK:O	88:Bz:404:UNK:HG3	2.13	0.49
1:AA:138:U:H5"	1:AA:139:A:N7	2.27	0.49
1:AA:928:A:H5'	1:AA:930:G:N7	2.28	0.49
2:AB:66:LEU:HD23	2:AB:133:HIS:CE1	2.48	0.49
6:AG:140:ASN:HB3	6:AG:143:THR:HG22	1.95	0.49
17:AY:55:Y5P:H6	17:AY:58:Y5P:C5	2.43	0.49
23:Ae:38:UNK:HA	23:Ae:41:UNK:CG	2.43	0.49
23:Ae:38:UNK:CA	23:Ae:41:UNK:HG3	2.42	0.49
23:Ae:398:UNK:C	23:Ae:401:UNK:HG3	2.42	0.49
29:Ak:194:LYS:HZ2	29:Ak:245:LYS:HZ2	1.60	0.49
32:Ao:598:UNK:O	32:Ao:602:UNK:HG3	2.13	0.49
33:Ap:68:TYR:HE2	33:Ap:73:VAL:HG13	1.78	0.49
33:Ap:89:ARG:HB2	33:Ap:144:MET:CE	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:B2:93:ARG:HH12	70:Be:83:PRO:HA	1.77	0.49
47:BB:38:P5P:H2'	47:BB:39:P5P:C8	2.43	0.49
49:BE:139:ASN:ND2	49:BE:141:ARG:HB2	2.28	0.49
52:BJ:101:HIS:CE1	52:BJ:109:LYS:HZ1	2.31	0.49
61:BU:122:ARG:NH1	62:BV:70:LEU:HG	2.28	0.49
66:Ba:128:LEU:HD13	66:Ba:376:VAL:HB	1.95	0.49
67:Bb:268:PHE:HE2	67:Bb:321:CYS:HB3	1.78	0.49
79:Bn:69:HIS:CD2	79:Bn:71:LYS:HG3	2.48	0.49
84:Bu:159:GLU:HG3	84:Bu:160:ALA:N	2.26	0.49
86:Bw:352:GLN:HB3	86:Bw:418:PHE:CE2	2.47	0.49
88:Bz:411:UNK:HA	88:Bz:414:UNK:HG3	1.93	0.49
1:AA:349:A:OP2	9:AK:121:ASN:ND2	2.45	0.49
1:AA:939:A:H2'	1:AA:940:C:C6	2.48	0.49
17:AY:8:Y5P:N3	17:AY:14:Y5P:H5	2.28	0.49
19:Aa:221:ASP:OD1	19:Aa:260:LEU:HD11	2.12	0.49
23:Ae:286:UNK:C	23:Ae:289:UNK:HG3	2.42	0.49
23:Ae:356:UNK:HG2	23:Ae:357:UNK:N	2.27	0.49
32:Ao:504:UNK:O	32:Ao:507:UNK:HG3	2.13	0.49
37:B1:113:GLU:HA	37:B1:123:PHE:O	2.12	0.49
46:BA:63:A:H3'	46:BA:64:C:O2	2.12	0.49
46:BA:506:G:H4'	53:BK:151:LEU:HD13	1.94	0.49
46:BA:524:A:O2'	53:BK:135:VAL:HG11	2.12	0.49
46:BA:715:A:H1'	66:Ba:266:GLN:HE21	1.78	0.49
46:BA:974:A:H5"	46:BA:975:G:OP2	2.13	0.49
46:BA:1354:C:H2'	46:BA:1355:C:O4'	2.13	0.49
46:BA:1399:U:C4	49:BE:242:ALA:HB2	2.48	0.49
49:BE:155:PHE:HA	68:Bc:305:HIS:CE1	2.48	0.49
49:BE:200:PRO:HA	49:BE:273:VAL:HG22	1.95	0.49
58:BR:129:ASN:ND2	58:BR:131:LEU:HB2	2.28	0.49
59:BS:102:VAL:HG12	59:BS:103:VAL:HG12	1.94	0.49
60:BT:229:TRP:CH2	60:BT:249:LEU:HD21	2.48	0.49
74:Bi:104:GLY:O	74:Bi:108:ARG:HG2	2.12	0.49
86:Bw:211:ILE:HD11	86:Bw:221:ASP:HB2	1.95	0.49
88:Bz:25:UNK:HA	88:Bz:28:UNK:HG3	1.95	0.49
1:AA:546:U:H2'	1:AA:547:A:C8	2.48	0.49
1:AA:882:A:N3	1:AA:886:A:N6	2.59	0.49
2:AB:166:HIS:ND1	7:AI:153:THR:HA	2.28	0.49
2:AB:240:ASP:HB2	24:Af:120:LYS:NZ	2.28	0.49
11:AN:103:ARG:HB3	11:AN:104:TRP:CZ3	2.48	0.49
21:Ac:27:VAL:HG21	21:Ac:106:LEU:HD13	1.93	0.49
24:Af:102:ILE:HD12	24:Af:174:GLN:OE1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Ag:82:LEU:HD12	25:Ag:83:PRO:HD2	1.94	0.49
37:B1:179:ASP:N	37:B1:179:ASP:OD1	2.44	0.49
38:B2:111:ARG:HG2	64:BX:25:PHE:CE1	2.47	0.49
46:BA:614:A:H5'	72:Bg:69:PRO:HB3	1.95	0.49
46:BA:1161:A:H2'	46:BA:1161:A:N3	2.27	0.49
46:BA:1230:G:C2'	46:BA:1246:C:H41	2.26	0.49
49:BE:347:PHE:HD1	60:BT:122:ALA:HB1	1.76	0.49
54:BN:159:THR:HG22	54:BN:161:GLU:H	1.76	0.49
57:BQ:106:ARG:HH11	57:BQ:106:ARG:CB	2.26	0.49
72:Bg:33:LEU:O	72:Bg:67:PRO:HA	2.12	0.49
78:Bm:86:ASN:OD1	78:Bm:86:ASN:N	2.44	0.49
1:AA:386:U:O2'	5:AF:93:ILE:O	2.31	0.48
1:AA:641:A:OP1	4:AE:230:ASN:HB2	2.12	0.48
1:AA:884:C:N4	23:Ae:103:UNK:O	2.44	0.48
5:AF:37:ARG:HA	22:Ad:167:PHE:CD1	2.48	0.48
12:AO:204:TRP:CZ2	12:AO:208:LYS:HD2	2.48	0.48
17:AV:28:Y5P:H2'	17:AV:29:Y5P:H6	1.95	0.48
22:Ad:117:HIS:CE1	22:Ad:121:LEU:HD11	2.48	0.48
23:Ae:219:UNK:O	23:Ae:222:UNK:HG3	2.13	0.48
23:Ae:294:UNK:O	23:Ae:297:UNK:CG	2.61	0.48
25:Ag:56:UNK:HB2	25:Ag:146:LYS:HZ1	1.77	0.48
25:Ag:150:LEU:HG	25:Ag:255:PHE:CE2	2.48	0.48
25:Ag:346:ASN:HB3	25:Ag:385:ARG:O	2.13	0.48
27:Ai:31:MET:O	27:Ai:34:VAL:HB	2.13	0.48
32:Ao:175:UNK:HA	32:Ao:178:UNK:HG3	1.95	0.48
32:Ao:188:UNK:HG2	32:Ao:189:UNK:N	2.27	0.48
32:Ao:355:UNK:O	32:Ao:358:UNK:CG	2.60	0.48
32:Ao:538:UNK:CG	32:Ao:550:UNK:HB2	2.39	0.48
33:Ap:126:PHE:CE2	33:Ap:140:THR:HG21	2.48	0.48
35:Az:693:UNK:O	35:Az:693:UNK:CG	2.60	0.48
39:B3:119:ILE:H	83:Bt:45:ASN:ND2	2.01	0.48
46:BA:375:A:O2'	46:BA:376:G:H5'	2.12	0.48
57:BQ:223:MET:HA	83:Bt:42:GLU:OE2	2.13	0.48
64:BX:138:ASP:HB3	64:BX:141:ARG:HB2	1.94	0.48
66:Ba:302:ARG:HH11	66:Ba:302:ARG:HG3	1.76	0.48
67:Bb:185:MET:SD	84:Bu:188:ARG:HB2	2.53	0.48
74:Bi:160:LEU:O	74:Bi:164:VAL:HG22	2.13	0.48
76:Bk:170:PHE:O	76:Bk:174:ILE:HG13	2.13	0.48
86:Bw:186:ASN:HA	86:Bw:422:ARG:NH2	2.28	0.48
1:AA:587:U:H5"	11:AN:33:LYS:NZ	2.28	0.48
1:AA:763:A:O3'	11:AN:58:ARG:NH2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AG:194:LYS:NZ	6:AG:218:PRO:HG2	2.29	0.48
19:Aa:154:LYS:NZ	19:Aa:181:ARG:NH2	2.61	0.48
19:Aa:281:ASP:OD2	19:Aa:337:UNK:HG3	2.12	0.48
22:Ad:54:PHE:HD2	33:Ap:208:PRO:HB3	1.78	0.48
23:Ae:75:UNK:HA	23:Ae:78:UNK:CG	2.44	0.48
24:Af:141:VAL:HB	24:Af:170:LEU:HD11	1.94	0.48
27:Ai:89:ARG:HG2	27:Ai:91:LYS:HG3	1.94	0.48
31:An:142:LYS:HD3	31:An:142:LYS:HA	1.49	0.48
32:Ao:374:UNK:HA	32:Ao:377:UNK:CG	2.42	0.48
32:Ao:599:UNK:HA	32:Ao:602:UNK:HG3	1.95	0.48
39:B3:86:ILE:HD12	39:B3:113:VAL:HG11	1.95	0.48
39:B3:122:LEU:HD12	39:B3:123:LYS:H	1.78	0.48
46:BA:945:A:C6	46:BA:946:A:N1	2.81	0.48
46:BA:1020:G:C5	46:BA:1021:U:C5	3.01	0.48
52:BJ:117:ARG:HG3	53:BK:134:ASP:HB3	1.95	0.48
65:BY:78:GLN:HE22	74:Bi:74:ARG:HE	1.60	0.48
67:Bb:194:THR:HB	67:Bb:197:GLU:OE1	2.13	0.48
83:Bt:18:ILE:HG22	83:Bt:19:GLY:N	2.28	0.48
87:Bx:99:MET:HE1	87:Bx:119:VAL:HG21	1.95	0.48
87:Bx:138:GLY:C	87:Bx:141:PRO:HD2	2.37	0.48
1:AA:54:A:H5"	22:Ad:28:LYS:HD2	1.96	0.48
1:AA:738:U:H2'	6:AG:198:ARG:HE	1.78	0.48
2:AB:133:HIS:O	2:AB:137:ARG:HG3	2.13	0.48
6:AG:89:PRO:HA	6:AG:92:SER:HB3	1.94	0.48
9:AK:151:VAL:HG11	9:AK:164:ILE:HD11	1.95	0.48
15:AR:133:ASP:HB3	15:AR:134:PRO:HD2	1.94	0.48
21:Ac:24:LYS:HZ2	21:Ac:107:GLY:H	1.60	0.48
23:Ae:130:UNK:O	23:Ae:130:UNK:HG3	2.14	0.48
23:Ae:399:UNK:CA	23:Ae:402:UNK:HG3	2.43	0.48
25:Ag:59:UNK:O	25:Ag:105:LEU:HD21	2.13	0.48
32:Ao:279:UNK:HG2	32:Ao:280:UNK:N	2.26	0.48
32:Ao:479:UNK:HA	32:Ao:482:UNK:HG3	1.94	0.48
37:B1:59:ARG:NH1	85:Bv:92:TRP:CD1	2.82	0.48
38:B2:160:THR:HG21	70:Be:129:TYR:HB2	1.95	0.48
46:BA:175:U:P	54:BN:115:ASN:HD22	2.36	0.48
46:BA:733:A:H2'	46:BA:734:C:O4'	2.13	0.48
46:BA:1006:A:H2'	46:BA:1006:A:N3	2.29	0.48
48:BD:115:GLU:H	48:BD:123:PHE:HZ	1.61	0.48
49:BE:205:ASP:OD2	49:BE:302:SER:HA	2.12	0.48
58:BR:53:ARG:HH21	58:BR:105:THR:HG22	1.78	0.48
59:BS:54:ARG:O	59:BS:58:LEU:HG	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:BT:71:PRO:HG2	60:BT:212:ASN:ND2	2.29	0.48
61:BU:100:LYS:HZ1	72:Bg:119:PHE:HE2	1.60	0.48
64:BX:14:ASN:ND2	65:BY:210:HIS:HA	2.28	0.48
67:Bb:40:ILE:HD11	76:Bk:62:LEU:HD21	1.95	0.48
70:Be:88:GLN:O	70:Be:92:GLU:HG2	2.13	0.48
86:Bw:195:ASP:O	86:Bw:233:ASN:HA	2.13	0.48
87:Bx:164:ASN:O	87:Bx:166:GLY:N	2.46	0.48
88:Bz:420:UNK:HG2	88:Bz:421:UNK:N	2.28	0.48
1:AA:109:G:H5”	10:AL:43:LYS:NZ	2.29	0.48
1:AA:159:C:H2’	1:AA:160:C:H5’	1.94	0.48
1:AA:787:A:H2’	1:AA:788:G:C8	2.49	0.48
3:AC:115:ASN:HD21	3:AC:150:PRO:HD2	1.79	0.48
4:AE:289:THR:HB	4:AE:307:LYS:HG3	1.95	0.48
8:AJ:179:GLN:O	29:Ak:150:PRO:HD2	2.13	0.48
14:AQ:57:GLN:NE2	14:AQ:57:GLN:O	2.46	0.48
14:AQ:74:THR:HG22	14:AQ:75:LYS:H	1.79	0.48
22:Ad:101:GLU:O	22:Ad:105:LEU:HG	2.12	0.48
23:Ae:149:UNK:O	23:Ae:153:UNK:HG2	2.13	0.48
23:Ae:378:UNK:O	23:Ae:382:UNK:HG2	2.13	0.48
32:Ao:172:UNK:HA	32:Ao:175:UNK:HG3	1.95	0.48
32:Ao:459:UNK:C	32:Ao:462:UNK:HG3	2.44	0.48
36:B0:77:PRO:HD2	59:BS:70:THR:OG1	2.12	0.48
38:B2:186:TRP:CD1	65:BY:216:TYR:CE2	3.02	0.48
46:BA:982:A:H2’	46:BA:983:C:O4’	2.14	0.48
46:BA:1399:U:O4	49:BE:242:ALA:HB2	2.13	0.48
46:BA:1550:C:H5’	46:BA:1551:A:OP1	2.13	0.48
49:BE:252:TRP:HE3	49:BE:253:PRO:HD2	1.78	0.48
56:BP:232:ALA:O	56:BP:235:GLU:HB3	2.13	0.48
67:Bb:224:HIS:CD2	67:Bb:227:GLU:H	2.32	0.48
69:Bd:154:SER:HB3	69:Bd:157:LEU:HD12	1.95	0.48
74:Bi:88:TYR:HD2	74:Bi:245:TYR:CE2	2.31	0.48
86:Bw:51:LEU:O	86:Bw:62:ARG:NE	2.33	0.48
1:AA:26:A:H2’	1:AA:27:U:C6	2.49	0.48
1:AA:254:C:H41	10:AL:74:ASN:HD22	1.61	0.48
9:AK:87:ILE:H	9:AK:87:ILE:HG13	1.42	0.48
23:Ae:75:UNK:O	23:Ae:78:UNK:HG3	2.14	0.48
32:Ao:190:UNK:HG1	32:Ao:223:UNK:CA	2.44	0.48
32:Ao:191:UNK:HA	32:Ao:194:UNK:CG	2.36	0.48
32:Ao:240:UNK:HA	32:Ao:243:UNK:HG3	1.96	0.48
36:B0:107:ASN:OD1	36:B0:108:PRO:HD2	2.14	0.48
46:BA:151:G:OP2	61:BU:37:ARG:NH1	2.35	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:BA:177:C:O2	61:BU:52:LYS:HD3	2.13	0.48
46:BA:378:U:O2'	56:BP:68:GLU:OE2	2.31	0.48
46:BA:1494:C:H5'	49:BE:220:ARG:HH12	1.78	0.48
52:BJ:136:GLU:HG2	52:BJ:144:LEU:HD11	1.95	0.48
53:BK:25:ARG:HA	53:BK:65:PRO:HB3	1.94	0.48
54:BN:80:HIS:CE1	54:BN:87:PHE:HB2	2.48	0.48
60:BT:168:ASN:OD1	60:BT:169:PRO:HD2	2.13	0.48
62:BV:60:LEU:HD22	87:Bx:187:TYR:HE1	1.78	0.48
63:BW:131:ASN:HB2	74:Bi:278:LYS:HZ3	1.77	0.48
65:BY:212:LYS:NZ	65:BY:214:TYR:HE1	2.11	0.48
73:Bh:148:LEU:HD12	73:Bh:152:GLY:HA3	1.96	0.48
1:AA:185:A:H1'	1:AA:214:U:O2	2.13	0.48
1:AA:194:U:H5'	13:AP:86:PRO:HG3	1.96	0.48
1:AA:529:G:H2'	1:AA:531:U:C5	2.48	0.48
4:AE:320:ILE:HD13	4:AE:349:LEU:HD13	1.96	0.48
19:Aa:208:ILE:HD13	19:Aa:229:LEU:HD11	1.95	0.48
23:Ae:267:UNK:CG	23:Ae:270:UNK:CG	2.89	0.48
25:Ag:301:GLN:NE2	29:Ak:270:GLN:OE1	2.44	0.48
32:Ao:421:UNK:HA	32:Ao:424:UNK:HG3	1.96	0.48
37:B1:224:ILE:H	37:B1:224:ILE:HG13	1.41	0.48
42:B6:26:THR:HB	46:BA:1239:U:H3'	1.96	0.48
46:BA:289:A:O2'	46:BA:792:A:OP1	2.32	0.48
46:BA:569:A:H3'	46:BA:570:A:H5"	1.96	0.48
46:BA:572:A:OP2	54:BN:68:SER:OG	2.27	0.48
46:BA:856:U:O4'	46:BA:858:G:H1'	2.13	0.48
46:BA:924:U:O2'	46:BA:925:A:O5'	2.29	0.48
49:BE:45:SER:O	68:Bc:303:ARG:NH2	2.47	0.48
50:BF:62:VAL:HG13	78:Bm:119:HIS:HB3	1.94	0.48
50:BF:216:VAL:HG22	50:BF:258:THR:HB	1.95	0.48
60:BT:74:ARG:HB3	60:BT:283:TRP:CZ2	2.48	0.48
66:Ba:153:ARG:NH1	66:Ba:187:LEU:HD22	2.25	0.48
67:Bb:261:ARG:NE	84:Bu:124:ASN:HD22	2.12	0.48
75:Bj:51:LEU:HD12	75:Bj:188:ALA:HB1	1.95	0.48
88:Bz:32:UNK:O	88:Bz:36:UNK:HG3	2.13	0.48
1:AA:605:C:H2'	1:AA:606:A:O4'	2.13	0.48
5:AF:6:LEU:HB3	5:AF:66:VAL:HB	1.94	0.48
6:AG:52:ARG:NH1	7:AI:361:GLU:OE2	2.23	0.48
17:AY:9:Y5P:C4	17:AY:22:Y5P:C5	2.92	0.48
19:Aa:340:UNK:HA	19:Aa:343:UNK:CG	2.43	0.48
23:Ae:67:UNK:HG3	23:Ae:68:UNK:N	2.29	0.48
23:Ae:256:UNK:HA	23:Ae:259:UNK:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Aj:27:ARG:HD2	28:Aj:28:PRO:HD2	1.94	0.48
29:Ak:153:ILE:HG12	29:Ak:221:TYR:CE1	2.49	0.48
30:Am:106:LYS:O	30:Am:110:ARG:HG3	2.14	0.48
32:Ao:373:UNK:O	32:Ao:376:UNK:HG3	2.12	0.48
36:B0:90:TYR:CZ	46:BA:1206:A:H4'	2.48	0.48
44:B8:98:SER:OG	44:B8:102:GLY:N	2.46	0.48
46:BA:237:C:C6	79:Bn:127:TYR:HB2	2.48	0.48
46:BA:416:G:O6	83:Bt:67:ARG:NH1	2.46	0.48
46:BA:501:A:H5'	46:BA:502:G:OP2	2.14	0.48
53:BK:17:SER:N	53:BK:72:VAL:O	2.46	0.48
66:Ba:201:ARG:NH1	66:Ba:418:TYR:O	2.40	0.48
66:Ba:387:TRP:HE1	66:Ba:404:ILE:HD11	1.78	0.48
67:Bb:284:ASP:N	67:Bb:284:ASP:OD1	2.46	0.48
68:Bc:266:ILE:HD12	68:Bc:271:ILE:HD12	1.96	0.48
86:Bw:163:ARG:HD3	86:Bw:163:ARG:HA	1.64	0.48
86:Bw:329:TRP:C	86:Bw:333:GLN:HE21	2.21	0.48
1:AA:800:G:H2'	1:AA:801:A:C8	2.48	0.48
2:AB:233:TYR:CE2	20:Ab:40:PRO:HB3	2.48	0.48
8:AJ:70:ASP:OD2	8:AJ:151:SER:OG	2.32	0.48
16:AU:83:PRO:HG2	16:AU:84:TRP:CD1	2.49	0.48
19:Aa:154:LYS:HZ3	19:Aa:181:ARG:NH2	2.12	0.48
23:Ae:46:UNK:HG2	23:Ae:48:UNK:HG3	1.95	0.48
23:Ae:112:UNK:O	23:Ae:115:UNK:HG3	2.13	0.48
28:Aj:78:ARG:NH2	28:Aj:144:LYS:HE3	2.29	0.48
28:Aj:165:PRO:HB2	33:Ap:199:TRP:CZ3	2.49	0.48
37:B1:156:LYS:NZ	37:B1:205:GLY:O	2.46	0.48
38:B2:143:ALA:O	38:B2:146:LYS:HB2	2.14	0.48
41:B5:91:ARG:HD3	46:BA:156:A:H4'	1.93	0.48
46:BA:63:A:H2'	46:BA:63:A:N3	2.29	0.48
46:BA:674:A:H5'	46:BA:675:C:OP2	2.14	0.48
46:BA:1368:U:H2'	46:BA:1369:C:H6	1.79	0.48
54:BN:178:LEU:HD21	87:Bx:100:LEU:HD11	1.94	0.48
60:BT:148:THR:HG22	60:BT:165:GLU:HA	1.96	0.48
66:Ba:173:ARG:HA	66:Ba:176:TYR:CE2	2.49	0.48
74:Bi:111:ARG:O	74:Bi:115:ASN:ND2	2.47	0.48
74:Bi:245:TYR:HB3	74:Bi:265:ILE:O	2.13	0.48
77:Bl:68:THR:HB	77:Bl:69:PRO:HD2	1.95	0.48
1:AA:201:A:H2'	1:AA:202:A:C8	2.49	0.48
1:AA:759:U:H2'	1:AA:760:A:H8	1.78	0.48
1:AA:768:A:H2'	1:AA:769:A:C8	2.49	0.48
1:AA:874:U:H3	1:AA:893:A:N6	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AG:119:LYS:HG3	6:AG:141:PRO:HD3	1.96	0.48
9:AK:90:ILE:HG12	9:AK:99:ILE:HG12	1.96	0.48
11:AN:125:ARG:HG2	11:AN:125:ARG:HH11	1.78	0.48
18:AX:17:Y5P:H4A	18:AX:18:Y5P:H4	1.95	0.48
22:Ad:199:ARG:HB3	22:Ad:200:PRO:HD2	1.94	0.48
23:Ae:218:UNK:CG	23:Ae:296:UNK:HG1	2.44	0.48
23:Ae:280:UNK:HA	23:Ae:283:UNK:HG3	1.95	0.48
30:Am:11:ALA:O	30:Am:12:ARG:NH1	2.37	0.48
30:Am:59:ASN:O	30:Am:62:ARG:HG2	2.13	0.48
32:Ao:394:UNK:HA	32:Ao:397:UNK:CG	2.42	0.48
39:B3:76:LYS:HB2	39:B3:76:LYS:HE3	1.56	0.48
41:B5:90:ASN:OD1	41:B5:93:ARG:NH2	2.46	0.48
48:BD:80:ARG:HE	48:BD:80:ARG:HB2	1.37	0.48
49:BE:145:LEU:HD23	49:BE:145:LEU:HA	1.64	0.48
50:BF:166:PRO:HG2	50:BF:169:VAL:HG21	1.95	0.48
50:BF:190:VAL:HG11	50:BF:193:LEU:HD13	1.96	0.48
58:BR:62:TYR:CE2	60:BT:269:MET:HE3	2.49	0.48
59:BS:54:ARG:HH12	59:BS:141:ILE:HG22	1.79	0.48
61:BU:149:ARG:HD2	71:Bf:56:ARG:NH2	2.28	0.48
66:Ba:329:TYR:HB3	66:Ba:334:LYS:HZ1	1.78	0.48
71:Bf:61:TYR:CD2	71:Bf:63:PRO:HD3	2.48	0.48
72:Bg:56:ARG:HG3	72:Bg:56:ARG:NH1	2.28	0.48
74:Bi:287:LEU:HD21	74:Bi:293:PHE:HD1	1.79	0.48
87:Bx:154:TRP:HE1	87:Bx:175:PRO:HG3	1.79	0.48
1:AA:194:U:H2'	1:AA:195:G:C8	2.49	0.48
1:AA:560:C:N4	1:AA:710:G:H1	2.11	0.48
19:Aa:314:UNK:CA	19:Aa:317:UNK:HG3	2.44	0.48
19:Aa:350:UNK:O	19:Aa:353:UNK:CG	2.49	0.48
25:Ag:59:UNK:CG	25:Ag:62:UNK:HB2	2.43	0.48
32:Ao:413:UNK:O	32:Ao:416:UNK:HG3	2.14	0.48
32:Ao:464:UNK:HA	32:Ao:467:UNK:HG3	1.96	0.48
32:Ao:484:UNK:C	32:Ao:487:UNK:HG3	2.44	0.48
39:B3:91:LEU:HA	39:B3:91:LEU:HD23	1.65	0.48
46:BA:420:U:H2'	46:BA:421:U:C6	2.49	0.48
46:BA:617:C:H2'	46:BA:618:A:C8	2.48	0.48
46:BA:1255:A:C8	46:BA:1255:A:C3'	2.97	0.48
49:BE:202:GLN:HB3	49:BE:273:VAL:HG13	1.96	0.48
53:BK:104:THR:HG21	53:BK:150:SER:C	2.39	0.48
61:BU:100:LYS:NZ	72:Bg:119:PHE:HE2	2.11	0.48
71:Bf:126:ARG:HH11	71:Bf:126:ARG:CG	2.22	0.48
73:Bh:32:LYS:HZ1	79:Bn:42:LYS:NZ	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:Bm:76:LYS:HG2	78:Bm:83:VAL:HG23	1.96	0.48
87:Bx:92:PHE:O	87:Bx:93:ILE:HG23	2.14	0.48
7:AI:104:ILE:O	7:AI:108:ILE:HG13	2.14	0.47
12:AO:210:LEU:HB2	31:An:189:TRP:CZ2	2.49	0.47
15:AR:55:MET:SD	15:AR:58:PRO:HG3	2.54	0.47
17:AY:55:Y5P:H5	17:AY:58:Y5P:H6	1.96	0.47
19:Aa:89:ILE:HD11	19:Aa:125:LEU:HD13	1.96	0.47
19:Aa:134:ARG:HD2	19:Aa:185:TRP:CD2	2.49	0.47
21:Ac:47:PHE:HA	21:Ac:51:ASN:ND2	2.29	0.47
23:Ae:83:UNK:HG2	23:Ae:84:UNK:N	2.29	0.47
23:Ae:93:UNK:HA	23:Ae:96:UNK:HG3	1.94	0.47
23:Ae:204:UNK:CB	23:Ae:223:UNK:HG2	2.38	0.47
23:Ae:296:UNK:CA	23:Ae:299:UNK:HG3	2.41	0.47
29:Ak:66:GLN:NE2	32:Ao:81:ASP:OD1	2.47	0.47
29:Ak:152:GLU:HG3	29:Ak:176:ARG:NH1	2.28	0.47
32:Ao:413:UNK:C	32:Ao:416:UNK:HG3	2.43	0.47
32:Ao:671:UNK:O	32:Ao:674:UNK:HG3	2.14	0.47
46:BA:164:A:H2'	46:BA:165:A:O4'	2.14	0.47
46:BA:624:G:C5	61:BU:11:ARG:HB2	2.49	0.47
56:BP:146:ASP:N	56:BP:146:ASP:OD1	2.44	0.47
58:BR:27:HIS:O	58:BR:30:GLN:HB2	2.14	0.47
59:BS:144:MET:O	59:BS:172:LEU:HA	2.14	0.47
63:BW:188:LYS:HB3	63:BW:192:ALA:HB3	1.95	0.47
67:Bb:261:ARG:HA	67:Bb:323:TRP:CG	2.49	0.47
67:Bb:267:ARG:HB3	67:Bb:320:GLN:NE2	2.29	0.47
79:Bn:105:ASP:OD1	79:Bn:105:ASP:N	2.45	0.47
1:AA:59:C:N4	28:Aj:133:GLN:HG2	2.14	0.47
1:AA:601:A:N6	27:Ai:63:GLY:HA3	2.29	0.47
5:AF:3:ARG:NH1	5:AF:4:TYR:CE1	2.76	0.47
17:AV:62:Y5P:C4	17:AV:63:Y5P:H4	2.43	0.47
23:Ae:137:UNK:HB2	28:Aj:72:PRO:HB3	1.95	0.47
25:Ag:150:LEU:HG	25:Ag:255:PHE:HE2	1.78	0.47
28:Aj:95:TRP:HE3	28:Aj:118:LEU:HD13	1.79	0.47
32:Ao:189:UNK:CA	32:Ao:192:UNK:HG3	2.42	0.47
41:B5:127:TYR:CE1	58:BR:110:ILE:HD11	2.49	0.47
44:B8:94:VAL:HG22	44:B8:161:MET:HG2	1.96	0.47
44:B8:149:PHE:CD2	67:Bb:358:PRO:HG2	2.49	0.47
46:BA:99:C:H5	79:Bn:75:LYS:NZ	2.11	0.47
46:BA:442:G:C6	52:BJ:31:LYS:NZ	2.80	0.47
46:BA:571:A:H4'	54:BN:30:LYS:HG3	1.96	0.47
46:BA:1036:A:OP2	71:Bf:121:HIS:HE1	1.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:BA:1053:A:H3'	50:BF:131:LYS:NZ	2.30	0.47
46:BA:1125:A:H2'	46:BA:1126:A:C8	2.49	0.47
46:BA:1264:U:H2'	46:BA:1265:A:C8	2.43	0.47
50:BF:192:SER:OG	50:BF:193:LEU:N	2.44	0.47
54:BN:3:SER:OG	73:Bh:308:THR:HG23	2.13	0.47
57:BQ:78:GLU:OE2	57:BQ:158:ARG:NH1	2.47	0.47
57:BQ:240:ARG:HG2	57:BQ:240:ARG:HH11	1.79	0.47
59:BS:104:SER:CB	67:Bb:150:ARG:HH22	2.27	0.47
66:Ba:283:TYR:CD1	66:Ba:284:PRO:HD2	2.49	0.47
69:Bd:151:ARG:HG2	69:Bd:158:HIS:HB3	1.96	0.47
69:Bd:168:LEU:HG	75:Bj:205:LEU:O	2.15	0.47
83:Bt:29:ALA:O	83:Bt:33:GLN:HG2	2.15	0.47
1:AA:104:A:OP2	14:AQ:49:TYR:OH	2.30	0.47
1:AA:647:A:H3'	1:AA:648:A:H5"	1.96	0.47
4:AE:307:LYS:HZ1	19:Aa:100:PRO:HG2	1.79	0.47
23:Ae:178:UNK:O	23:Ae:182:UNK:HG2	2.15	0.47
23:Ae:288:UNK:C	23:Ae:291:UNK:HG3	2.44	0.47
25:Ag:259:VAL:HB	25:Ag:305:ILE:HG22	1.96	0.47
32:Ao:309:UNK:HG2	32:Ao:310:UNK:N	2.30	0.47
32:Ao:433:UNK:HA	32:Ao:436:UNK:HG3	1.96	0.47
46:BA:14:C:O2'	50:BF:111:TYR:HB3	2.14	0.47
46:BA:150:A:H8	46:BA:150:A:O5'	1.96	0.47
46:BA:355:G:C2	46:BA:356:U:C2	3.03	0.47
46:BA:1253:A:H2'	46:BA:1254:C:H6	1.79	0.47
49:BE:194:TYR:HB3	49:BE:281:ASN:HD21	1.79	0.47
49:BE:215:PHE:CE2	49:BE:259:GLY:HA2	2.48	0.47
51:BI:57:GLU:HG2	51:BI:58:ARG:N	2.29	0.47
56:BP:281:LYS:HD2	77:Bl:40:GLU:HG2	1.96	0.47
61:BU:83:TYR:CZ	61:BU:87:ILE:HG13	2.49	0.47
62:BV:140:VAL:O	62:BV:146:THR:HG23	2.14	0.47
66:Ba:213:TRP:NE1	66:Ba:215:ARG:HB2	2.28	0.47
68:Bc:140:TRP:CZ3	68:Bc:176:PHE:HD2	2.31	0.47
72:Bg:101:VAL:HA	72:Bg:104:LEU:HD12	1.96	0.47
73:Bh:141:PHE:HB2	73:Bh:153:VAL:HG23	1.95	0.47
74:Bi:88:TYR:HB3	74:Bi:245:TYR:OH	2.13	0.47
74:Bi:122:ILE:HD13	74:Bi:134:ILE:HG13	1.96	0.47
1:AA:520:G:C2	1:AA:521:G:N7	2.83	0.47
1:AA:708:A:OP1	1:AA:708:A:H4'	2.15	0.47
4:AE:154:VAL:HG22	32:Ao:108:LEU:HD21	1.96	0.47
12:AO:90:VAL:HG13	22:Ad:160:LEU:HD23	1.96	0.47
12:AO:178:VAL:O	12:AO:182:ILE:HG12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AQ:16:LYS:O	14:AQ:29:ARG:N	2.43	0.47
23:Ae:120:UNK:O	23:Ae:120:UNK:HG2	2.13	0.47
28:Aj:38:TYR:OH	28:Aj:63:ARG:NH2	2.47	0.47
29:Ak:112:ASN:HB2	29:Ak:114:LEU:HG	1.96	0.47
32:Ao:300:UNK:HA	32:Ao:303:UNK:CG	2.44	0.47
32:Ao:581:UNK:HG1	32:Ao:654:UNK:HG3	1.86	0.47
32:Ao:654:UNK:O	32:Ao:657:UNK:HG3	2.14	0.47
32:Ao:659:UNK:HB2	32:Ao:670:UNK:CG	2.44	0.47
36:B0:76:HIS:CG	59:BS:70:THR:HG21	2.49	0.47
36:B0:92:LEU:HA	36:B0:92:LEU:HD23	1.53	0.47
43:B7:88:LYS:HG2	46:BA:117:G:C8	2.49	0.47
45:B9:71:LYS:NZ	46:BA:494:C:H5'	2.29	0.47
46:BA:357:U:H6	46:BA:357:U:H5"	1.79	0.47
46:BA:522:C:C5	46:BA:530:A:H5"	2.50	0.47
46:BA:714:A:H5'	48:BD:71:LYS:NZ	2.29	0.47
46:BA:1201:C:O2'	56:BP:77:ARG:NH1	2.47	0.47
49:BE:104:LEU:HD23	49:BE:104:LEU:HA	1.63	0.47
50:BF:97:HIS:ND1	56:BP:27:LEU:HB3	2.29	0.47
57:BQ:83:THR:OG1	57:BQ:123:ARG:NH1	2.48	0.47
63:BW:78:ILE:HG22	63:BW:80:TYR:H	1.79	0.47
63:BW:201:LEU:HB3	63:BW:204:ARG:HH21	1.79	0.47
64:BX:88:LYS:HE3	70:Be:20:LYS:HE2	1.96	0.47
68:Bc:112:MET:HB2	68:Bc:267:PRO:HB3	1.97	0.47
84:Bu:182:MET:HE2	84:Bu:182:MET:HB3	1.85	0.47
85:Bv:65:GLY:HA2	85:Bv:68:SER:HB3	1.96	0.47
1:AA:522:A:H2'	1:AA:523:C:O4'	2.13	0.47
2:AB:213:LYS:HG3	20:Ab:5:ARG:O	2.15	0.47
8:AJ:83:HIS:CE1	11:AN:122:GLY:HA3	2.50	0.47
12:AO:69:PRO:HD2	12:AO:72:MET:HG3	1.95	0.47
49:BE:175:LYS:HB3	49:BE:296:LEU:HD23	1.95	0.47
51:BI:84:GLU:HG3	51:BI:85:ASP:N	2.28	0.47
57:BQ:71:ASP:OD1	57:BQ:72:ILE:HG13	2.14	0.47
74:Bi:102:LYS:HD2	74:Bi:102:LYS:HA	1.66	0.47
75:Bj:172:MET:HE3	75:Bj:174:PRO:HA	1.97	0.47
86:Bw:315:GLU:OE2	86:Bw:319:ARG:NH2	2.48	0.47
1:AA:438:C:H2'	1:AA:439:A:O4'	2.14	0.47
1:AA:899:C:O3'	1:AA:900:A:H4'	2.15	0.47
3:AC:87:VAL:HG11	27:Ai:53:PRO:HG2	1.96	0.47
7:AI:198:SER:HA	7:AI:247:ARG:O	2.14	0.47
11:AN:62:ILE:HG12	26:Ah:341:HIS:ND1	2.30	0.47
15:AR:86:SER:HA	15:AR:93:TYR:OH	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AY:28:Y5P:O5'	17:AY:28:Y5P:H6	2.14	0.47
21:Ac:12:THR:HG22	21:Ac:14:GLN:H	1.80	0.47
21:Ac:125:HIS:CD2	21:Ac:127:ALA:HB3	2.50	0.47
25:Ag:59:UNK:HG1	25:Ag:62:UNK:HG1	1.97	0.47
25:Ag:120:ALA:O	25:Ag:298:ASN:HB2	2.14	0.47
26:Ah:358:VAL:O	26:Ah:362:VAL:HG23	2.15	0.47
28:Aj:78:ARG:HD2	28:Aj:141:LEU:HD21	1.96	0.47
32:Ao:384:UNK:HG2	32:Ao:385:UNK:N	2.29	0.47
32:Ao:413:UNK:HA	32:Ao:416:UNK:CG	2.42	0.47
32:Ao:659:UNK:HG1	32:Ao:670:UNK:HG2	1.95	0.47
37:B1:197:PRO:HG2	37:B1:200:GLU:HG3	1.97	0.47
38:B2:190:TRP:HB3	65:BY:216:TYR:CE1	2.49	0.47
44:B8:132:LYS:O	44:B8:136:LYS:HG3	2.15	0.47
46:BA:388:A:H1'	77:Bl:104:ASN:ND2	2.30	0.47
46:BA:521:U:O2'	46:BA:522:C:O5'	2.29	0.47
49:BE:123:GLN:HG2	49:BE:124:VAL:O	2.15	0.47
54:BN:128:PHE:HA	54:BN:129:PRO:HD3	1.71	0.47
59:BS:68:TRP:C	59:BS:70:THR:H	2.23	0.47
67:Bb:265:PHE:CZ	67:Bb:322:ARG:HD2	2.49	0.47
69:Bd:166:PRO:HA	69:Bd:169:PHE:CE1	2.50	0.47
75:Bj:64:THR:HB	75:Bj:67:GLN:HG3	1.97	0.47
86:Bw:157:ALA:N	86:Bw:158:PRO:HD2	2.30	0.47
86:Bw:241:LEU:HD22	86:Bw:242:PRO:HD2	1.97	0.47
87:Bx:79:HIS:HA	87:Bx:184:ASN:HD22	1.79	0.47
1:AA:31:U:OP1	10:AL:134:HIS:HE1	1.97	0.47
1:AA:168:A:O2'	1:AA:170:A:N1	2.47	0.47
1:AA:256:G:O6	18:AX:21:Y5P:HC	2.13	0.47
1:AA:815:U:OP1	7:AI:278:LYS:HG2	2.14	0.47
92:AA:8113:HOH:O	17:AV:30:Y5P:C4	2.52	0.47
2:AB:168:ARG:HH22	16:AU:87:CYS:C	2.23	0.47
4:AE:256:PHE:CZ	4:AE:347:ARG:HG2	2.49	0.47
6:AG:194:LYS:NZ	6:AG:218:PRO:HB2	2.30	0.47
7:AI:202:ILE:HG13	7:AI:205:GLU:HG3	1.95	0.47
7:AI:316:PHE:HB3	7:AI:317:PRO:HD3	1.97	0.47
9:AK:154:LYS:HA	9:AK:180:ASN:O	2.14	0.47
11:AN:33:LYS:HB3	11:AN:90:ARG:NH2	2.30	0.47
17:AV:24:Y5P:C4	17:AV:25:Y5P:H4	2.43	0.47
19:Aa:324:UNK:HG2	19:Aa:325:UNK:N	2.29	0.47
23:Ae:87:UNK:HA	60:BT:60:UNK:HG1	1.96	0.47
23:Ae:122:UNK:CG	23:Ae:123:UNK:N	2.77	0.47
23:Ae:170:UNK:CG	28:Aj:78:ARG:NH2	2.74	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Ae:174:UNK:HG2	23:Ae:176:UNK:N	2.29	0.47
23:Ae:360:UNK:HA	23:Ae:363:UNK:HG3	1.97	0.47
25:Ag:55:UNK:CG	25:Ag:56:UNK:N	2.71	0.47
25:Ag:79:PRO:HG2	25:Ag:193:ALA:HA	1.97	0.47
25:Ag:356:ILE:HG21	25:Ag:376:LYS:HD2	1.95	0.47
26:Ah:352:LYS:HA	29:Ak:213:ARG:HB3	1.96	0.47
32:Ao:266:UNK:O	32:Ao:270:UNK:HG3	2.14	0.47
32:Ao:280:UNK:C	32:Ao:283:UNK:HG3	2.44	0.47
32:Ao:376:UNK:O	32:Ao:379:UNK:HG3	2.15	0.47
32:Ao:516:UNK:O	32:Ao:519:UNK:HG3	2.14	0.47
38:B2:115:LEU:HB3	64:BX:27:GLN:HG2	1.97	0.47
39:B3:63:PRO:HA	83:Bt:51:ARG:HH12	1.78	0.47
44:B8:101:LYS:HE3	46:BA:75:A:C2	2.48	0.47
46:BA:777:G:C2	46:BA:778:G:H1'	2.50	0.47
46:BA:809:A:N3	49:BE:230:THR:HG21	2.30	0.47
46:BA:890:G:H2'	46:BA:891:U:H6	1.80	0.47
46:BA:1494:C:H5'	49:BE:220:ARG:NH1	2.29	0.47
46:BA:1551:A:H3'	46:BA:1552:G:H8	1.79	0.47
48:BD:165:LEU:HB3	48:BD:181:ASP:OD1	2.14	0.47
49:BE:187:ILE:HG22	49:BE:188:LYS:N	2.29	0.47
49:BE:275:ARG:HD2	49:BE:333:TYR:CE1	2.49	0.47
54:BN:176:TYR:CE2	87:Bx:104:ILE:HG13	2.50	0.47
55:BO:40:VAL:HA	55:BO:105:VAL:HG23	1.97	0.47
56:BP:157:GLN:HA	56:BP:177:ALA:O	2.14	0.47
59:BS:79:HIS:CE1	67:Bb:154:TYR:OH	2.67	0.47
59:BS:176:ARG:HG2	59:BS:177:ARG:H	1.78	0.47
62:BV:112:VAL:HG13	62:BV:199:ILE:HG21	1.97	0.47
65:BY:172:ASP:HB3	65:BY:176:ASP:HB2	1.97	0.47
66:Ba:149:ASN:OD1	66:Ba:149:ASN:N	2.48	0.47
67:Bb:53:SER:HG	67:Bb:56:ARG:H	1.63	0.47
69:Bd:157:LEU:HD11	75:Bj:178:TRP:HZ2	1.79	0.47
70:Be:126:PHE:HB3	70:Be:133:PHE:CD1	2.50	0.47
71:Bf:116:PHE:HD1	73:Bh:267:LEU:HD21	1.80	0.47
74:Bi:93:GLY:O	74:Bi:97:ILE:HG13	2.15	0.47
77:Bl:76:ARG:HB2	77:Bl:78:PRO:O	2.15	0.47
84:Bu:182:MET:HA	84:Bu:185:GLU:HB2	1.97	0.47
86:Bw:213:ARG:HB2	86:Bw:213:ARG:CZ	2.44	0.47
88:Bz:28:UNK:HA	88:Bz:31:UNK:CG	2.39	0.47
88:Bz:404:UNK:CG	88:Bz:405:UNK:N	2.77	0.47
88:Bz:405:UNK:HA	88:Bz:408:UNK:HG3	1.95	0.47
19:Aa:131:LEU:HD11	33:Ap:177:PHE:CD1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Aa:322:UNK:HG3	19:Aa:325:UNK:CG	2.44	0.47
25:Ag:135:LEU:HD12	25:Ag:138:CYS:HB3	1.96	0.47
32:Ao:220:UNK:HA	32:Ao:223:UNK:CG	2.45	0.47
41:B5:84:ARG:HB2	46:BA:1010:U:O2	2.15	0.47
46:BA:120:C:H2'	46:BA:121:C:H6	1.79	0.47
46:BA:197:U:H2'	46:BA:198:A:H8	1.80	0.47
53:BK:66:LEU:HB3	53:BK:85:PRO:HG3	1.96	0.47
57:BQ:124:VAL:HA	57:BQ:158:ARG:NH2	2.28	0.47
64:BX:150:LEU:HG	74:Bi:240:ARG:HG2	1.95	0.47
65:BY:59:GLY:H	65:BY:76:VAL:HB	1.80	0.47
75:Bj:210:CYS:SG	75:Bj:235:LYS:HB2	2.55	0.47
85:Bv:44:ASP:OD1	85:Bv:45:PRO:HD2	2.15	0.47
88:Bz:304:UNK:HA	88:Bz:307:UNK:HG3	1.96	0.47
88:Bz:606:UNK:HA	88:Bz:609:UNK:CG	2.43	0.47
1:AA:287:C:N3	21:Ac:11:ARG:NH2	2.63	0.47
2:AB:140:ILE:HG23	2:AB:164:TYR:CD2	2.50	0.47
5:AF:3:ARG:HG2	5:AF:4:TYR:CE1	2.50	0.47
8:AJ:81:LYS:HE2	8:AJ:140:TYR:HE1	1.80	0.47
10:AL:69:LYS:HZ3	10:AL:77:ASN:HB3	1.79	0.47
19:Aa:106:THR:HG22	19:Aa:107:GLN:H	1.80	0.47
20:Ab:12:ILE:HG22	20:Ab:15:ARG:HH12	1.80	0.47
21:Ac:7:PHE:O	21:Ac:10:ARG:HG2	2.14	0.47
23:Ae:79:UNK:HG1	23:Ae:88:UNK:HB1	1.96	0.47
23:Ae:82:UNK:O	23:Ae:82:UNK:HG2	2.14	0.47
32:Ao:268:UNK:O	32:Ao:272:UNK:HG3	2.15	0.47
32:Ao:379:UNK:O	32:Ao:382:UNK:HG3	2.14	0.47
32:Ao:412:UNK:HG2	32:Ao:413:UNK:N	2.30	0.47
32:Ao:510:UNK:CG	32:Ao:511:UNK:N	2.78	0.47
39:B3:142:ASN:OD1	39:B3:144:GLU:HB3	2.15	0.47
46:BA:76:G:N2	46:BA:88:G:H2'	2.30	0.47
46:BA:85:A:C5	46:BA:86:U:H1'	2.49	0.47
46:BA:440:A:H5'	57:BQ:66:ARG:HB2	1.96	0.47
46:BA:488:U:H5	87:Bx:173:ARG:NH2	2.12	0.47
46:BA:799:G:H4'	55:BO:36:THR:HG22	1.97	0.47
46:BA:1328:U:H2'	46:BA:1329:G:O4'	2.15	0.47
52:BJ:95:MET:HE3	52:BJ:164:MET:SD	2.55	0.47
53:BK:43:GLY:HA3	53:BK:76:ARG:NH1	2.24	0.47
55:BO:57:CYS:SG	55:BO:58:ILE:N	2.88	0.47
55:BO:96:MET:HG2	60:BT:164:PHE:CD1	2.49	0.47
59:BS:44:VAL:HA	67:Bb:225:LEU:HB3	1.96	0.47
60:BT:99:MET:HE3	60:BT:167:TYR:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:BX:2:ALA:HB2	64:BX:19:VAL:HG11	1.96	0.47
68:Bc:66:HIS:HB3	68:Bc:74:THR:HB	1.97	0.47
68:Bc:106:ASP:OD1	68:Bc:106:ASP:N	2.48	0.47
85:Bv:146:UNK:O	85:Bv:149:UNK:HG3	2.14	0.47
88:Bz:12:UNK:HG2	88:Bz:13:UNK:N	2.30	0.47
1:AA:234:A:N6	1:AA:250:A:N1	2.62	0.47
3:AC:144:SER:HA	3:AC:149:CYS:O	2.15	0.47
20:Ab:73:LYS:HZ3	20:Ab:114:GLU:CD	2.23	0.47
25:Ag:122:ARG:HH11	25:Ag:336:LEU:HD22	1.80	0.47
25:Ag:162:LYS:HB3	25:Ag:315:LEU:HD11	1.97	0.47
25:Ag:201:ILE:HG12	25:Ag:255:PHE:CE1	2.50	0.47
32:Ao:283:UNK:HA	32:Ao:286:UNK:HG3	1.96	0.47
32:Ao:306:UNK:O	32:Ao:306:UNK:HG2	2.14	0.47
35:Az:705:UNK:HG2	35:Az:706:UNK:N	2.30	0.47
39:B3:72:ILE:CD1	39:B3:118:ARG:HD3	2.45	0.47
41:B5:157:VAL:HA	58:BR:130:CYS:SG	2.55	0.47
46:BA:224:C:OP1	56:BP:132:SER:OG	2.33	0.47
46:BA:438:A:OP1	57:BQ:73:ARG:NH2	2.48	0.47
46:BA:521:U:HO2'	46:BA:522:C:C5'	2.28	0.47
46:BA:733:A:OP2	48:BD:103:ARG:NH2	2.48	0.47
46:BA:787:A:O2'	49:BE:215:PHE:O	2.24	0.47
46:BA:895:A:H2'	46:BA:896:C:C6	2.50	0.47
46:BA:960:U:H2'	46:BA:961:G:C8	2.50	0.47
46:BA:1044:A:C2	46:BA:1435:A:C2	3.03	0.47
50:BF:69:LEU:HD22	50:BF:193:LEU:HD12	1.97	0.47
56:BP:39:ARG:O	56:BP:41:ARG:N	2.45	0.47
58:BR:108:LEU:HD11	58:BR:136:LEU:HD22	1.97	0.47
67:Bb:308:GLN:HE22	80:Bo:111:LYS:H	1.63	0.47
73:Bh:161:THR:HG23	73:Bh:196:PHE:CZ	2.50	0.47
86:Bw:158:PRO:C	86:Bw:160:ILE:H	2.22	0.47
1:AA:317:A:C2	1:AA:318:C:C5	3.03	0.46
1:AA:535:U:H2'	1:AA:536:C:O4'	2.15	0.46
1:AA:606:A:O2'	11:AN:28:TYR:OH	2.16	0.46
1:AA:959:U:H4'	1:AA:960:A:O5'	2.15	0.46
2:AB:146:ARG:HG2	2:AB:205:HIS:CD2	2.49	0.46
8:AJ:109:HIS:CE1	8:AJ:142:CYS:HB3	2.50	0.46
9:AK:160:ARG:HH12	16:AU:27:ASN:HD21	1.62	0.46
17:AV:48:Y5P:OP2	17:AV:48:Y5P:H6	2.15	0.46
17:AY:54:Y5P:H4A	17:AY:55:Y5P:C5	2.45	0.46
23:Ae:128:UNK:CG	23:Ae:129:UNK:N	2.78	0.46
23:Ae:362:UNK:O	23:Ae:365:UNK:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Ag:264:VAL:HG23	25:Ag:308:THR:O	2.15	0.46
25:Ag:325:GLN:HE22	29:Ak:302:LYS:HD3	1.80	0.46
32:Ao:194:UNK:HA	32:Ao:230:UNK:CG	2.28	0.46
32:Ao:301:UNK:O	32:Ao:304:UNK:HG3	2.15	0.46
47:BB:9:P5P:H1'	47:BB:46:P5P:C2	2.45	0.46
49:BE:90:TRP:HA	49:BE:316:PHE:CE2	2.47	0.46
53:BK:149:ARG:HH12	82:Bq:104:PRO:HD3	1.80	0.46
59:BS:65:GLU:OE2	67:Bb:74:TYR:OH	2.33	0.46
61:BU:69:ILE:O	61:BU:73:THR:OG1	2.27	0.46
63:BW:85:MET:HG3	63:BW:145:SER:OG	2.15	0.46
63:BW:152:LYS:HD3	63:BW:164:ILE:HD11	1.97	0.46
64:BX:150:LEU:HD21	74:Bi:274:GLN:HB2	1.97	0.46
66:Ba:203:CYS:HB3	86:Bw:173:GLN:HE22	1.80	0.46
75:Bj:55:ARG:NH1	75:Bj:157:LEU:HD22	2.29	0.46
78:Bm:67:LEU:O	78:Bm:71:LEU:HD12	2.14	0.46
1:AA:348:A:OP2	9:AK:122:ALA:HB2	2.15	0.46
1:AA:456:A:OP2	1:AA:952:C:O2'	2.30	0.46
6:AG:113:GLN:OE1	6:AG:202:PRO:HG2	2.15	0.46
19:Aa:154:LYS:NZ	19:Aa:181:ARG:HH22	2.13	0.46
19:Aa:348:UNK:HA	19:Aa:351:UNK:CG	2.43	0.46
22:Ad:166:THR:O	22:Ad:176:ARG:NH2	2.49	0.46
25:Ag:328:LEU:HB3	25:Ag:332:GLY:HA3	1.97	0.46
32:Ao:401:UNK:O	32:Ao:405:UNK:HG3	2.14	0.46
33:Ap:237:GLU:HG2	33:Ap:238:VAL:N	2.30	0.46
37:B1:202:GLU:HG3	37:B1:203:TRP:CD1	2.50	0.46
46:BA:163:A:H2'	46:BA:163:A:N3	2.30	0.46
46:BA:220:A:N7	50:BF:281:THR:OG1	2.41	0.46
49:BE:96:ARG:HH12	49:BE:301:ASP:CG	2.20	0.46
59:BS:72:TRP:CG	59:BS:73:PRO:HA	2.50	0.46
70:Be:66:PHE:CE2	70:Be:68:LEU:HB2	2.51	0.46
77:Bl:86:VAL:HB	77:Bl:166:PHE:HB3	1.97	0.46
78:Bm:70:ARG:HH11	78:Bm:109:LEU:HD23	1.80	0.46
88:Bz:18:UNK:CG	88:Bz:19:UNK:N	2.77	0.46
1:AA:256:G:OP1	1:AA:257:U:H5'	2.14	0.46
8:AJ:179:GLN:HA	29:Ak:149:PHE:HA	1.96	0.46
23:Ae:207:UNK:HG3	23:Ae:220:UNK:HB1	1.97	0.46
25:Ag:348:ASN:HB2	25:Ag:349:PRO:HD2	1.97	0.46
28:Aj:92:PRO:HD3	28:Aj:153:UNK:HG2	1.95	0.46
37:B1:21:TYR:HE2	37:B1:208:LEU:HD21	1.80	0.46
37:B1:65:VAL:HG22	51:BI:71:PRO:HG2	1.98	0.46
37:B1:202:GLU:HG3	37:B1:203:TRP:HD1	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:B6:26:THR:CG2	85:Bv:117:ARG:HH12	2.20	0.46
44:B8:96:TYR:N	44:B8:96:TYR:CD1	2.84	0.46
46:BA:292:U:HO2'	46:BA:1432:U:HO2'	1.62	0.46
46:BA:473:A:N6	46:BA:594:A:C6	2.83	0.46
52:BJ:95:MET:HB3	52:BJ:156:SER:HB2	1.96	0.46
56:BP:114:GLN:HB3	56:BP:115:PRO:HD2	1.97	0.46
61:BU:91:ILE:O	61:BU:94:GLN:N	2.44	0.46
66:Ba:387:TRP:NE1	66:Ba:404:ILE:HD11	2.30	0.46
68:Bc:156:LYS:HB3	68:Bc:159:TYR:HD2	1.80	0.46
71:Bf:78:UNK:O	71:Bf:78:UNK:CG	2.62	0.46
1:AA:259:A:O2'	1:AA:260:U:H5"	2.15	0.46
1:AA:439:A:H5'	1:AA:440:C:OP2	2.15	0.46
1:AA:498:U:H5'	1:AA:499:C:OP2	2.16	0.46
2:AB:137:ARG:HD3	20:Ab:34:ILE:HD11	1.98	0.46
2:AB:164:TYR:CD1	7:AI:149:PHE:HA	2.51	0.46
2:AB:203:GLU:OE2	30:Am:114:LYS:NZ	2.48	0.46
5:AF:6:LEU:HG	5:AF:8:LEU:HG	1.96	0.46
5:AF:97:PRO:HG3	15:AR:76:LYS:HZ2	1.79	0.46
23:Ae:251:UNK:O	23:Ae:255:UNK:CG	2.58	0.46
23:Ae:367:UNK:C	23:Ae:370:UNK:HG3	2.45	0.46
39:B3:76:LYS:HZ3	46:BA:472:G:H8	1.56	0.46
40:B4:55:VAL:HG21	40:B4:69:TYR:HB3	1.97	0.46
43:B7:93:LEU:HD22	43:B7:93:LEU:HA	1.85	0.46
46:BA:69:C:N4	85:Bv:49:ARG:CZ	2.78	0.46
46:BA:488:U:H5	87:Bx:173:ARG:HH21	1.62	0.46
46:BA:833:A:HO2'	46:BA:1428:G:HO2'	1.61	0.46
46:BA:1072:U:H3'	46:BA:1073:U:H5"	1.98	0.46
46:BA:1202:A:C2	46:BA:1203:G:H1'	2.50	0.46
46:BA:1557:A:H4'	49:BE:263:ASN:ND2	2.29	0.46
52:BJ:63:ARG:HH11	87:Bx:108:CYS:HA	1.79	0.46
60:BT:224:MET:HB2	60:BT:248:CYS:SG	2.55	0.46
61:BU:65:ARG:HA	61:BU:68:TRP:CE3	2.50	0.46
63:BW:134:PHE:HB3	68:Bc:90:MET:HB3	1.96	0.46
78:Bm:116:SER:O	78:Bm:119:HIS:ND1	2.42	0.46
85:Bv:142:ARG:CA	85:Bv:145:UNK:HG3	2.43	0.46
86:Bw:170:PHE:CZ	86:Bw:174:LEU:HD22	2.50	0.46
1:AA:185:A:O2'	1:AA:213:G:N2	2.48	0.46
1:AA:914:A:H2'	1:AA:915:G:O4'	2.16	0.46
4:AE:391:LEU:HD21	19:Aa:107:GLN:HB2	1.97	0.46
5:AF:92:ASN:CG	15:AR:118:LEU:HD22	2.40	0.46
6:AG:62:GLU:HG2	6:AG:66:ARG:HE	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AI:129:GLU:HG3	7:AI:130:GLU:HG3	1.98	0.46
9:AK:181:THR:O	9:AK:183:ILE:HG13	2.14	0.46
13:AP:100:HIS:ND1	13:AP:101:PRO:HD2	2.30	0.46
15:AR:56:GLU:CD	15:AR:56:GLU:H	2.22	0.46
21:Ac:15:TYR:HA	21:Ac:18:GLN:HG2	1.98	0.46
23:Ae:181:UNK:CG	23:Ae:210:UNK:HG3	2.34	0.46
23:Ae:221:UNK:CA	23:Ae:224:UNK:HG3	2.44	0.46
23:Ae:232:UNK:HG1	23:Ae:235:UNK:CG	2.35	0.46
23:Ae:390:UNK:CA	23:Ae:393:UNK:HG3	2.45	0.46
31:An:146:LEU:CD1	31:An:149:ARG:HH12	2.29	0.46
37:B1:94:ASN:HD21	51:BI:81:LYS:HB2	1.80	0.46
46:BA:226:U:HO2'	46:BA:229:G:H4'	1.80	0.46
46:BA:378:U:OP2	56:BP:62:ARG:NH1	2.48	0.46
46:BA:392:A:C2	46:BA:418:A:C2	3.03	0.46
46:BA:485:A:H61	46:BA:580:C:H42	1.63	0.46
49:BE:66:SER:O	49:BE:69:ASN:HB2	2.15	0.46
55:BO:60:VAL:HG22	55:BO:62:ASN:H	1.80	0.46
57:BQ:172:VAL:HA	57:BQ:175:PHE:CE2	2.50	0.46
59:BS:133:ALA:HB1	59:BS:168:GLY:HA3	1.98	0.46
66:Ba:211:ALA:HB3	66:Ba:222:VAL:HG13	1.97	0.46
66:Ba:280:GLN:HG3	86:Bw:150:PHE:HA	1.97	0.46
76:Bk:166:PHE:O	76:Bk:170:PHE:HB2	2.16	0.46
87:Bx:164:ASN:O	87:Bx:165:LYS:C	2.57	0.46
1:AA:485:G:H2'	1:AA:486:C:O4'	2.16	0.46
2:AB:87:ARG:HG3	2:AB:243:PRO:HG2	1.96	0.46
4:AE:98:LEU:HD11	27:Ai:75:HIS:CD2	2.51	0.46
7:AI:276:LYS:HE3	7:AI:281:LYS:HE2	1.98	0.46
10:AL:32:THR:OG1	10:AL:35:GLN:HG3	2.16	0.46
13:AP:67:ALA:HB2	19:Aa:195:TYR:CE2	2.50	0.46
15:AR:104:LYS:HD3	15:AR:104:LYS:HA	1.59	0.46
17:AV:58:Y5P:H6	17:AV:58:Y5P:H2'	1.74	0.46
23:Ae:173:UNK:HA	23:Ae:177:UNK:HG2	1.96	0.46
23:Ae:236:UNK:O	23:Ae:239:UNK:HG3	2.14	0.46
23:Ae:284:UNK:HA	23:Ae:287:UNK:HG3	1.96	0.46
26:Ah:345:LEU:HD11	27:Ai:26:THR:HG21	1.97	0.46
29:Ak:301:LEU:HA	29:Ak:310:THR:HG21	1.97	0.46
32:Ao:298:UNK:O	32:Ao:302:UNK:HB1	2.15	0.46
33:Ap:68:TYR:CE2	33:Ap:73:VAL:HG13	2.50	0.46
41:B5:119:LYS:NZ	49:BE:46:VAL:O	2.47	0.46
46:BA:493:A:OP1	46:BA:557:A:N6	2.49	0.46
46:BA:913:C:O5'	46:BA:913:C:H6	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:BA:1232:U:H5'	56:BP:79:PRO:HB3	1.98	0.46
49:BE:74:ALA:O	49:BE:77:LEU:HB3	2.14	0.46
49:BE:90:TRP:CH2	49:BE:312:LYS:HE2	2.51	0.46
55:BO:96:MET:HE1	60:BT:170:ARG:HD3	1.98	0.46
55:BO:107:LEU:HA	55:BO:107:LEU:HD23	1.61	0.46
66:Ba:60:TYR:CZ	66:Ba:73:PRO:HD3	2.50	0.46
67:Bb:351:HIS:HA	67:Bb:352:PRO:HD3	1.80	0.46
68:Bc:140:TRP:HH2	68:Bc:296:LEU:HD12	1.81	0.46
73:Bh:159:PHE:HD2	73:Bh:160:LEU:HD23	1.80	0.46
73:Bh:216:ARG:HB2	73:Bh:220:ILE:HD12	1.97	0.46
74:Bi:142:LYS:O	74:Bi:146:ILE:HG13	2.15	0.46
74:Bi:288:LYS:HD2	74:Bi:290:TRP:CZ2	2.51	0.46
75:Bj:61:LYS:HG2	75:Bj:154:ASP:HB2	1.98	0.46
75:Bj:198:ASN:HB2	75:Bj:242:ASP:O	2.16	0.46
86:Bw:324:ALA:O	86:Bw:327:PHE:HB3	2.16	0.46
86:Bw:416:VAL:O	86:Bw:420:LEU:HB2	2.16	0.46
87:Bx:176:VAL:HG21	87:Bx:196:HIS:NE2	2.30	0.46
1:AA:615:A:C6	1:AA:691:G:C5	3.03	0.46
4:AE:200:GLY:O	4:AE:221:ARG:HD2	2.16	0.46
4:AE:215:TYR:HB3	4:AE:218:PHE:HD2	1.81	0.46
5:AF:9:ILE:HD11	15:AR:118:LEU:O	2.16	0.46
7:AI:341:GLN:O	7:AI:345:VAL:HG23	2.15	0.46
11:AN:93:MET:H	11:AN:93:MET:HG2	1.40	0.46
19:Aa:280:ILE:HG22	19:Aa:284:LEU:HG	1.97	0.46
19:Aa:300:VAL:HG13	19:Aa:330:UNK:HG1	1.94	0.46
23:Ae:365:UNK:HG2	23:Ae:368:UNK:HG2	1.98	0.46
25:Ag:194:ASN:HB2	25:Ag:197:PHE:HD2	1.79	0.46
25:Ag:209:TRP:CH2	25:Ag:224:VAL:HG13	2.51	0.46
25:Ag:210:ASN:ND2	25:Ag:231:ARG:HH11	2.13	0.46
28:Aj:36:LEU:HD13	28:Aj:43:ARG:NE	2.31	0.46
32:Ao:484:UNK:HA	32:Ao:487:UNK:HG3	1.98	0.46
37:B1:91:TYR:CD2	51:BI:79:VAL:HG11	2.51	0.46
39:B3:41:ILE:HA	39:B3:42:PRO:HD2	1.68	0.46
46:BA:168:U:O4	71:Bf:135:LYS:NZ	2.44	0.46
46:BA:396:C:C4	46:BA:397:A:C2	3.04	0.46
46:BA:767:A:H5"	46:BA:767:A:H8	1.80	0.46
46:BA:841:C:H4'	48:BD:258:ILE:HG22	1.97	0.46
46:BA:975:G:N7	92:BA:1882:HOH:O	2.36	0.46
46:BA:1139:A:H2'	46:BA:1140:U:H6	1.78	0.46
46:BA:1491:A:C5	58:BR:14:VAL:HG21	2.50	0.46
55:BO:69:VAL:HG12	55:BO:127:LEU:HD21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:BO:91:MET:HG2	55:BO:92:PRO:HD2	1.97	0.46
60:BT:260:TRP:O	60:BT:262:GLN:HG3	2.15	0.46
65:BY:149:ARG:HD3	65:BY:150:SER:OG	2.16	0.46
68:Bc:45:PHE:CD2	68:Bc:253:ARG:NH1	2.80	0.46
71:Bf:126:ARG:CG	71:Bf:126:ARG:NH1	2.78	0.46
71:Bf:135:LYS:HE3	71:Bf:135:LYS:HB2	1.76	0.46
73:Bh:199:ILE:HD13	73:Bh:199:ILE:HA	1.80	0.46
75:Bj:192:LEU:HD23	75:Bj:192:LEU:HA	1.85	0.46
76:Bk:178:LEU:HA	76:Bk:179:PRO:HD3	1.76	0.46
81:Bp:81:LEU:HD13	81:Bp:86:MET:HG2	1.98	0.46
84:Bu:76:LEU:HD13	84:Bu:100:VAL:HG13	1.98	0.46
84:Bu:97:LYS:HE2	84:Bu:97:LYS:HB2	1.58	0.46
2:AB:180:LEU:HD12	2:AB:180:LEU:HA	1.77	0.46
4:AE:180:ASP:O	4:AE:184:LYS:HG2	2.16	0.46
5:AF:105:CYS:HB3	15:AR:69:CYS:SG	2.55	0.46
10:AL:32:THR:O	10:AL:36:MET:HG3	2.16	0.46
17:AY:38:Y5P:H4A	17:AY:39:Y5P:C4	2.45	0.46
19:Aa:291:ASP:OD1	19:Aa:348:UNK:HG2	2.16	0.46
23:Ae:118:UNK:O	23:Ae:119:UNK:CG	2.63	0.46
23:Ae:149:UNK:O	23:Ae:153:UNK:CG	2.64	0.46
43:B7:77:THR:HA	43:B7:80:GLN:HG3	1.98	0.46
46:BA:72:U:C4	46:BA:73:A:N7	2.84	0.46
46:BA:1301:C:H2'	46:BA:1302:G:H5'	1.98	0.46
46:BA:1409:G:H2'	46:BA:1410:A:O4'	2.16	0.46
54:BN:45:PRO:HD2	72:Bg:130:TRP:CZ2	2.51	0.46
57:BQ:39:PHE:HB3	57:BQ:42:VAL:HG23	1.98	0.46
57:BQ:127:PRO:HA	57:BQ:152:THR:OG1	2.15	0.46
64:BX:26:ILE:HD12	64:BX:56:TYR:CE1	2.51	0.46
66:Ba:135:LYS:HD2	66:Ba:239:VAL:HG12	1.97	0.46
76:Bk:100:MET:HE3	76:Bk:153:HIS:ND1	2.31	0.46
1:AA:704:U:H2'	1:AA:705:G:C8	2.50	0.46
4:AE:372:GLU:HB2	19:Aa:102:TYR:CE2	2.51	0.46
14:AQ:95:VAL:HG11	22:Ad:120:ARG:NH2	2.27	0.46
21:Ac:25:ASP:OD1	21:Ac:25:ASP:N	2.49	0.46
21:Ac:140:MET:HG3	21:Ac:143:VAL:HB	1.98	0.46
22:Ad:158:LEU:O	22:Ad:162:GLU:HG2	2.16	0.46
23:Ae:359:UNK:HA	23:Ae:362:UNK:CG	2.46	0.46
28:Aj:95:TRP:CE3	28:Aj:118:LEU:HD13	2.50	0.46
32:Ao:605:UNK:CG	32:Ao:651:UNK:CG	2.94	0.46
36:B0:40:LYS:HB2	36:B0:40:LYS:HE3	1.57	0.46
37:B1:157:PHE:CE2	66:Ba:48:ARG:NH1	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:BA:203:G:N1	56:BP:49:CYS:SG	2.89	0.46
46:BA:289:A:C2	46:BA:301:A:C2	3.03	0.46
46:BA:446:A:N7	46:BA:448:C:C2	2.83	0.46
46:BA:1030:G:H2'	46:BA:1031:G:C8	2.51	0.46
46:BA:1339:A:H2'	46:BA:1339:A:N3	2.30	0.46
46:BA:1382:A:H2'	46:BA:1383:U:O4'	2.16	0.46
46:BA:1547:A:C2	71:Bf:104:GLU:HG2	2.51	0.46
49:BE:212:GLY:O	58:BR:11:HIS:CE1	2.69	0.46
50:BF:103:GLN:HE22	50:BF:250:VAL:H	1.64	0.46
50:BF:283:LEU:HD23	50:BF:284:TYR:CE2	2.51	0.46
59:BS:125:CYS:SG	59:BS:157:SER:HB2	2.56	0.46
59:BS:130:ARG:HH11	67:Bb:129:ARG:NH1	2.14	0.46
67:Bb:45:LEU:O	67:Bb:50:LYS:NZ	2.49	0.46
68:Bc:70:THR:O	68:Bc:72:PRO:HD3	2.16	0.46
69:Bd:99:ARG:H	69:Bd:99:ARG:HD3	1.81	0.46
73:Bh:314:TRP:HD1	73:Bh:315:ASP:O	1.98	0.46
78:Bm:106:ALA:HA	78:Bm:111:HIS:O	2.16	0.46
84:Bu:60:ARG:HD3	84:Bu:60:ARG:HA	1.54	0.46
88:Bz:414:UNK:O	88:Bz:417:UNK:HG3	2.15	0.46
1:AA:752:A:H3'	1:AA:753:A:H5'	1.98	0.46
1:AA:768:A:H2'	1:AA:769:A:H8	1.81	0.46
1:AA:891:C:C5	28:Aj:21:LEU:HD11	2.51	0.46
2:AB:164:TYR:HD1	7:AI:149:PHE:HA	1.81	0.46
4:AE:130:GLN:HB2	27:Ai:72:ARG:NH2	2.31	0.46
5:AF:105:CYS:HA	15:AR:103:LYS:NZ	2.31	0.46
11:AN:125:ARG:HG2	11:AN:125:ARG:NH1	2.31	0.46
21:Ac:158:GLU:HA	21:Ac:163:TYR:CD1	2.50	0.46
23:Ae:279:UNK:CG	23:Ae:280:UNK:N	2.79	0.46
26:Ah:341:HIS:CD2	27:Ai:24:ARG:HD2	2.51	0.46
31:An:132:LYS:HE3	31:An:132:LYS:HB2	1.84	0.46
32:Ao:222:UNK:HA	32:Ao:225:UNK:CG	2.46	0.46
32:Ao:493:UNK:HG2	32:Ao:494:UNK:N	2.30	0.46
33:Ap:105:CYS:HB3	33:Ap:106:PRO:HD2	1.97	0.46
43:B7:82:ILE:HG23	43:B7:93:LEU:HD13	1.97	0.46
46:BA:63:A:OP2	92:BA:1924:HOH:O	2.21	0.46
46:BA:220:A:H5"	46:BA:221:G:OP2	2.16	0.46
46:BA:924:U:O2'	46:BA:925:A:C8	2.67	0.46
46:BA:1036:A:OP2	71:Bf:121:HIS:CE1	2.68	0.46
55:BO:118:ARG:HA	55:BO:140:ILE:HB	1.98	0.46
62:BV:114:ALA:O	62:BV:115:GLU:HB2	2.16	0.46
66:Ba:136:VAL:HG22	66:Ba:420:HIS:CD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:Bb:279:ILE:HD12	67:Bb:311:MET:HE3	1.97	0.46
70:Be:68:LEU:HD12	70:Be:68:LEU:HA	1.84	0.46
70:Be:91:LEU:O	70:Be:96:PRO:HD3	2.14	0.46
88:Bz:26:UNK:C	88:Bz:29:UNK:HG3	2.45	0.46
1:AA:287:C:OP2	14:AQ:38:TYR:OH	2.31	0.45
1:AA:757:U:H2'	1:AA:758:U:O4'	2.15	0.45
6:AG:200:LEU:HD22	6:AG:200:LEU:HA	1.79	0.45
7:AI:376:ARG:HG3	7:AI:376:ARG:HH11	1.81	0.45
15:AR:65:LYS:HB3	15:AR:69:CYS:CB	2.47	0.45
19:Aa:105:MET:HE2	19:Aa:109:GLN:HB3	1.97	0.45
19:Aa:310:UNK:HG3	19:Aa:313:UNK:CB	2.46	0.45
23:Ae:255:UNK:O	23:Ae:259:UNK:HB1	2.16	0.45
25:Ag:347:TYR:CZ	25:Ag:387:PRO:HB3	2.51	0.45
31:An:196:LEU:O	31:An:198:ASN:ND2	2.49	0.45
32:Ao:190:UNK:HG1	32:Ao:223:UNK:CB	2.43	0.45
32:Ao:502:UNK:HA	32:Ao:505:UNK:HG3	1.99	0.45
46:BA:69:C:HO2'	46:BA:70:A:P	2.35	0.45
46:BA:960:U:H2'	46:BA:961:G:H8	1.80	0.45
46:BA:1159:G:H2'	46:BA:1160:G:H8	1.81	0.45
46:BA:1312:U:O2'	46:BA:1313:U:O4'	2.34	0.45
50:BF:103:GLN:HE22	50:BF:250:VAL:N	2.14	0.45
57:BQ:89:ILE:HG13	57:BQ:161:VAL:HB	1.97	0.45
58:BR:93:LEU:HD12	58:BR:93:LEU:HA	1.68	0.45
59:BS:79:HIS:NE2	67:Bb:154:TYR:OH	2.48	0.45
62:BV:113:THR:O	62:BV:199:ILE:HG12	2.16	0.45
66:Ba:355:LEU:HD12	66:Ba:356:VAL:N	2.31	0.45
67:Bb:240:ILE:HG23	67:Bb:244:ARG:O	2.15	0.45
69:Bd:150:LEU:HB2	75:Bj:212:HIS:CE1	2.51	0.45
74:Bi:247:VAL:HG12	74:Bi:262:HIS:HB3	1.99	0.45
75:Bj:161:VAL:HA	75:Bj:251:HIS:O	2.16	0.45
83:Bt:9:ARG:CG	83:Bt:9:ARG:NH1	2.76	0.45
86:Bw:303:GLU:OE2	86:Bw:307:LYS:HG3	2.15	0.45
86:Bw:347:ARG:H	86:Bw:347:ARG:HG3	1.64	0.45
1:AA:950:U:H2'	1:AA:951:G:C8	2.51	0.45
17:AV:70:Y5P:H4A	17:AV:71:Y5P:H4	1.98	0.45
23:Ae:111:UNK:HA	23:Ae:114:UNK:HG3	1.97	0.45
23:Ae:114:UNK:HA	23:Ae:117:UNK:CG	2.40	0.45
23:Ae:182:UNK:O	23:Ae:186:UNK:HG2	2.15	0.45
27:Ai:46:LYS:HA	27:Ai:49:TYR:CE2	2.52	0.45
29:Ak:151:ILE:HG12	29:Ak:177:VAL:HG22	1.99	0.45
32:Ao:457:UNK:HG2	32:Ao:458:UNK:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:B3:125:PRO:HG2	39:B3:144:GLU:HG3	1.97	0.45
42:B6:38:ARG:NH2	42:B6:39:GLU:OE1	2.49	0.45
44:B8:98:SER:HG	44:B8:102:GLY:N	2.14	0.45
46:BA:566:C:N4	46:BA:567:C:N3	2.64	0.45
46:BA:718:C:OP1	46:BA:718:C:H6	2.00	0.45
46:BA:1264:U:C2	46:BA:1265:A:C8	3.04	0.45
49:BE:116:LYS:C	49:BE:117:HIS:HD1	2.24	0.45
49:BE:202:GLN:O	49:BE:272:LYS:HA	2.16	0.45
50:BF:284:TYR:HB2	50:BF:285:PRO:HD2	1.97	0.45
57:BQ:183:LEU:HD23	57:BQ:183:LEU:HA	1.75	0.45
62:BV:60:LEU:HB2	87:Bx:80:LYS:O	2.17	0.45
62:BV:91:ILE:HG22	62:BV:206:PRO:HA	1.98	0.45
63:BW:57:TYR:HD2	63:BW:67:ARG:NH1	2.14	0.45
66:Ba:60:TYR:OH	66:Ba:72:ARG:HD3	2.16	0.45
71:Bf:126:ARG:HA	71:Bf:126:ARG:HD2	1.64	0.45
71:Bf:129:TYR:OH	71:Bf:133:ARG:NH1	2.48	0.45
72:Bg:60:GLY:O	73:Bh:78:ARG:NH1	2.49	0.45
73:Bh:262:GLY:HA3	73:Bh:265:THR:OG1	2.16	0.45
75:Bj:264:LEU:HG	75:Bj:269:LEU:HB3	1.97	0.45
84:Bu:166:UNK:O	84:Bu:167:UNK:CG	2.58	0.45
86:Bw:203:PHE:HB2	86:Bw:226:GLN:OE1	2.17	0.45
1:AA:629:C:H2'	1:AA:630:A:H8	1.80	0.45
1:AA:825:C:HO2'	1:AA:826:C:P	2.39	0.45
2:AB:97:ARG:HH12	20:Ab:60:VAL:HG11	1.81	0.45
2:AB:217:PRO:HG3	20:Ab:31:TRP:HB2	1.98	0.45
8:AJ:109:HIS:NE2	8:AJ:142:CYS:HB3	2.32	0.45
8:AJ:183:HIS:CE1	35:Az:708:UNK:CG	2.99	0.45
18:AX:20:Y5P:H4A	18:AX:21:Y5P:H4	1.99	0.45
19:Aa:77:ILE:HG21	19:Aa:302:LEU:HG	1.98	0.45
19:Aa:240:GLU:OE1	19:Aa:243:LYS:NZ	2.48	0.45
21:Ac:28:LYS:O	21:Ac:62:VAL:HG13	2.17	0.45
23:Ae:79:UNK:CG	23:Ae:88:UNK:HB1	2.45	0.45
28:Aj:29:ARG:HG3	28:Aj:31:SER:H	1.82	0.45
29:Ak:291:VAL:O	29:Ak:295:ARG:HG3	2.17	0.45
32:Ao:204:UNK:CA	32:Ao:207:UNK:HG3	2.38	0.45
37:B1:27:HIS:CD2	37:B1:28:TYR:N	2.85	0.45
44:B8:183:ARG:NH1	67:Bb:354:GLN:NE2	2.64	0.45
46:BA:187:C:C4	46:BA:1023:A:N1	2.84	0.45
46:BA:1194:G:OP2	67:Bb:368:ARG:NH1	2.50	0.45
46:BA:1258:U:H2'	46:BA:1259:U:H6	1.81	0.45
46:BA:1348:G:H1	46:BA:1357:C:H42	1.62	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:BB:37:P5P:H8	47:BB:37:P5P:OP2	2.15	0.45
48:BD:126:LYS:HB2	66:Ba:258:PRO:HG2	1.97	0.45
53:BK:29:ALA:HB3	53:BK:54:ASN:ND2	2.31	0.45
56:BP:142:GLU:N	56:BP:142:GLU:OE1	2.49	0.45
63:BW:57:TYR:CD2	63:BW:67:ARG:NH1	2.84	0.45
65:BY:153:ILE:O	65:BY:153:ILE:HG13	2.15	0.45
69:Bd:97:LYS:HD3	75:Bj:84:TYR:CE2	2.52	0.45
73:Bh:102:GLU:HA	73:Bh:105:ARG:HB3	1.99	0.45
73:Bh:274:LEU:O	73:Bh:281:ILE:HG12	2.16	0.45
76:Bk:81:ASN:HB3	76:Bk:86:TYR:CE2	2.52	0.45
79:Bn:88:LEU:HD13	79:Bn:117:LEU:HB3	1.99	0.45
86:Bw:237:ILE:HD11	86:Bw:290:HIS:CG	2.51	0.45
88:Bz:24:UNK:HA	88:Bz:27:UNK:HG3	1.98	0.45
3:AC:43:ARG:HD3	3:AC:43:ARG:HA	1.74	0.45
3:AC:100:PHE:CE2	3:AC:155:LEU:HD21	2.51	0.45
4:AE:324:CYS:HB3	4:AE:329:ILE:HB	1.99	0.45
5:AF:105:CYS:HB2	15:AR:70:GLU:H	1.81	0.45
9:AK:195:ARG:HD3	9:AK:195:ARG:HA	1.53	0.45
11:AN:80:ARG:O	11:AN:86:ARG:HD2	2.16	0.45
12:AO:172:ARG:NH1	14:AQ:88:VAL:HG21	2.31	0.45
22:Ad:30:ARG:HE	22:Ad:30:ARG:HB2	1.54	0.45
23:Ae:256:UNK:HA	23:Ae:259:UNK:CG	2.47	0.45
25:Ag:115:ASN:HB3	25:Ag:118:HIS:CD2	2.52	0.45
32:Ao:121:ILE:HG22	32:Ao:142:PRO:HB3	1.98	0.45
32:Ao:157:UNK:O	32:Ao:161:UNK:HB1	2.17	0.45
32:Ao:269:UNK:HA	32:Ao:272:UNK:HG3	1.98	0.45
32:Ao:304:UNK:C	32:Ao:307:UNK:HG3	2.43	0.45
32:Ao:497:UNK:HA	32:Ao:500:UNK:CG	2.46	0.45
33:Ap:136:HIS:HD2	33:Ap:139:TYR:H	1.64	0.45
43:B7:57:GLN:O	46:BA:253:G:H8	1.99	0.45
46:BA:48:U:H1'	51:BI:78:ARG:HH12	1.80	0.45
46:BA:54:A:H5"	46:BA:55:A:OP2	2.16	0.45
46:BA:93:U:H5'	56:BP:196:ARG:HD3	1.98	0.45
46:BA:216:A:O2'	46:BA:218:A:H4'	2.17	0.45
46:BA:481:G:H2'	46:BA:482:U:O4'	2.17	0.45
46:BA:1045:A:O4'	49:BE:244:SER:HB3	2.16	0.45
46:BA:1535:A:H2'	46:BA:1536:A:O4'	2.17	0.45
52:BJ:63:ARG:HH12	87:Bx:108:CYS:HA	1.81	0.45
57:BQ:53:VAL:HG21	57:BQ:102:PHE:HB3	1.99	0.45
60:BT:118:ARG:HA	60:BT:133:PHE:O	2.16	0.45
62:BV:100:PHE:HD2	72:Bg:126:ILE:HD12	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:BX:15:PRO:HA	65:BY:208:ARG:NH1	2.32	0.45
73:Bh:35:PHE:HE1	73:Bh:39:TYR:CD1	2.35	0.45
73:Bh:252:ALA:O	73:Bh:254:GLU:HG3	2.17	0.45
76:Bk:113:LEU:HD23	76:Bk:170:PHE:HE1	1.81	0.45
86:Bw:340:TRP:CH2	86:Bw:342:GLU:HB2	2.51	0.45
86:Bw:369:ASN:H	86:Bw:385:ASN:ND2	2.11	0.45
88:Bz:417:UNK:CG	88:Bz:418:UNK:N	2.79	0.45
1:AA:348:A:P	9:AK:122:ALA:HB2	2.56	0.45
1:AA:526:G:N2	1:AA:840:A:C4	2.84	0.45
1:AA:861:A:C6	1:AA:908:A:C6	3.04	0.45
3:AC:76:LEU:HD22	8:AJ:138:THR:HG23	1.97	0.45
16:AU:46:GLU:OE2	16:AU:54:ARG:NH1	2.49	0.45
23:Ae:45:UNK:HG2	23:Ae:45:UNK:O	2.16	0.45
23:Ae:225:UNK:O	23:Ae:229:UNK:HG3	2.16	0.45
23:Ae:294:UNK:C	23:Ae:297:UNK:HG3	2.46	0.45
25:Ag:111:LEU:HA	25:Ag:114:THR:HG23	1.98	0.45
32:Ao:335:UNK:HA	32:Ao:365:UNK:HG2	1.98	0.45
32:Ao:362:UNK:O	32:Ao:366:UNK:HB1	2.17	0.45
32:Ao:375:UNK:HA	32:Ao:378:UNK:CG	2.47	0.45
32:Ao:496:UNK:O	32:Ao:500:UNK:HB1	2.16	0.45
37:B1:25:PRO:HB2	37:B1:27:HIS:CE1	2.51	0.45
42:B6:43:LEU:O	42:B6:55:LEU:HA	2.17	0.45
46:BA:1052:A:C5	46:BA:1324:A:C2	3.05	0.45
49:BE:199:ARG:HH11	49:BE:199:ARG:CG	2.29	0.45
57:BQ:42:VAL:HG21	57:BQ:166:ARG:HA	1.97	0.45
59:BS:127:SER:O	59:BS:131:VAL:HG23	2.15	0.45
60:BT:168:ASN:ND2	60:BT:170:ARG:HB2	2.31	0.45
62:BV:180:LYS:O	62:BV:181:ARG:HG2	2.17	0.45
64:BX:141:ARG:HD2	64:BX:141:ARG:HA	1.64	0.45
65:BY:59:GLY:N	65:BY:76:VAL:O	2.49	0.45
66:Ba:200:ARG:HH11	66:Ba:233:LYS:CD	2.26	0.45
68:Bc:285:THR:HG22	68:Bc:286:GLN:H	1.82	0.45
83:Bt:57:GLU:H	83:Bt:57:GLU:HG3	1.44	0.45
86:Bw:352:GLN:HB3	86:Bw:418:PHE:CD2	2.52	0.45
87:Bx:94:ARG:HH21	87:Bx:101:PRO:HD3	1.80	0.45
1:AA:180:U:H2'	1:AA:181:A:H8	1.80	0.45
1:AA:232:G:O6	1:AA:250:A:N6	2.50	0.45
1:AA:665:A:H62	8:AJ:85:LYS:HE3	1.82	0.45
1:AA:826:C:H2'	1:AA:827:A:C8	2.46	0.45
4:AE:289:THR:HG21	4:AE:308:GLN:N	2.31	0.45
4:AE:380:LEU:HD13	19:Aa:86:LEU:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AF:75:VAL:HA	5:AF:78:MET:SD	2.56	0.45
14:AQ:55:LEU:H	14:AQ:55:LEU:HG	1.53	0.45
19:Aa:144:ASP:N	19:Aa:144:ASP:OD1	2.46	0.45
19:Aa:340:UNK:CA	19:Aa:343:UNK:HG3	2.45	0.45
22:Ad:149:TRP:CZ2	22:Ad:153:LYS:HE3	2.52	0.45
23:Ae:120:UNK:O	23:Ae:124:UNK:CG	2.62	0.45
23:Ae:398:UNK:CA	23:Ae:401:UNK:HG3	2.42	0.45
25:Ag:197:PHE:O	25:Ag:201:ILE:HG13	2.16	0.45
32:Ao:202:UNK:HA	32:Ao:205:UNK:HB1	1.98	0.45
32:Ao:316:UNK:HG2	32:Ao:317:UNK:N	2.30	0.45
37:B1:91:TYR:HE2	51:BI:79:VAL:HG11	1.79	0.45
38:B2:123:ARG:NH1	64:BX:30:ARG:HB3	2.32	0.45
44:B8:103:LYS:NZ	46:BA:76:G:OP2	2.43	0.45
46:BA:104:C:H5”	46:BA:105:G:OP1	2.17	0.45
46:BA:444:A:OP1	52:BJ:35:ARG:NH2	2.36	0.45
46:BA:532:A:H5”	82:Bq:134:LYS:NZ	2.32	0.45
46:BA:669:C:OP1	70:Be:28:ARG:N	2.43	0.45
51:BI:130:VAL:HB	51:BI:136:ASN:HD21	1.80	0.45
56:BP:205:LEU:HD23	56:BP:205:LEU:HA	1.74	0.45
58:BR:16:ARG:HG2	58:BR:51:GLU:OE1	2.16	0.45
58:BR:150:LEU:HD23	68:Bc:312:LEU:HD21	1.98	0.45
59:BS:133:ALA:O	59:BS:136:CYS:HB2	2.16	0.45
61:BU:137:GLU:HB2	61:BU:138:PRO:HD3	1.98	0.45
62:BV:60:LEU:HA	62:BV:60:LEU:HD23	1.78	0.45
68:Bc:199:PHE:HB3	68:Bc:277:VAL:HG21	1.98	0.45
69:Bd:83:ILE:HG22	88:Bz:399:UNK:HA	1.98	0.45
69:Bd:119:LYS:O	69:Bd:122:SER:OG	2.31	0.45
69:Bd:147:LEU:O	69:Bd:151:ARG:HG3	2.17	0.45
75:Bj:85:SER:HB3	75:Bj:88:GLU:HB2	1.98	0.45
87:Bx:151:LEU:HD22	87:Bx:177:GLY:HA2	1.98	0.45
88:Bz:307:UNK:HA	88:Bz:310:UNK:HG3	1.97	0.45
1:AA:202:A:N1	22:Ad:46:PRO:HG2	2.31	0.45
1:AA:792:U:H2’	1:AA:793:A:H8	1.80	0.45
2:AB:158:ALA:HB2	2:AB:165:ALA:HB2	1.99	0.45
8:AJ:132:VAL:HG21	11:AN:112:ARG:NH1	2.31	0.45
22:Ad:117:HIS:CE1	22:Ad:121:LEU:HD21	2.51	0.45
23:Ae:200:UNK:CG	23:Ae:226:UNK:CG	2.93	0.45
29:Ak:167:ASN:HA	29:Ak:168:PRO:HD2	1.80	0.45
46:BA:15:A:H2’	46:BA:16:A:C8	2.49	0.45
46:BA:755:A:C5	86:Bw:215:HIS:HA	2.52	0.45
46:BA:1349:U:OP2	46:BA:1349:U:H6	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:BQ:101:HIS:O	57:BQ:105:MET:HG3	2.16	0.45
59:BS:177:ARG:HD3	59:BS:180:GLU:HG3	1.97	0.45
71:Bf:119:THR:HG23	71:Bf:121:HIS:H	1.82	0.45
79:Bn:62:ILE:HA	79:Bn:66:PHE:CE2	2.51	0.45
86:Bw:187:PRO:HD2	86:Bw:422:ARG:HH22	1.81	0.45
86:Bw:221:ASP:OD1	86:Bw:222:ALA:N	2.50	0.45
87:Bx:162:ILE:H	87:Bx:162:ILE:HG13	1.68	0.45
88:Bz:9:UNK:O	88:Bz:13:UNK:HG3	2.17	0.45
1:AA:368:A:O5'	9:AK:186:ASN:ND2	2.50	0.45
4:AE:303:ILE:HD12	4:AE:303:ILE:HA	1.76	0.45
10:AL:64:ARG:HG3	10:AL:66:PHE:HD2	1.82	0.45
12:AO:99:ALA:HB1	12:AO:103:GLU:HG3	1.98	0.45
13:AP:54:TYR:CD1	13:AP:66:VAL:HG22	2.47	0.45
16:AU:67:GLU:HB3	30:Am:29:LEU:HD11	1.98	0.45
19:Aa:198:ARG:HB3	19:Aa:201:ARG:HD2	1.99	0.45
19:Aa:312:UNK:HB1	19:Aa:333:UNK:HB2	1.99	0.45
23:Ae:69:UNK:HA	23:Ae:72:UNK:CG	2.47	0.45
23:Ae:359:UNK:CA	23:Ae:362:UNK:HG3	2.47	0.45
25:Ag:160:TRP:CD1	25:Ag:182:GLU:HG2	2.52	0.45
32:Ao:374:UNK:O	32:Ao:378:UNK:CG	2.55	0.45
32:Ao:476:UNK:HB1	32:Ao:506:UNK:CG	2.46	0.45
32:Ao:497:UNK:O	32:Ao:501:UNK:HG3	2.17	0.45
32:Ao:548:UNK:HG2	32:Ao:549:UNK:N	2.31	0.45
35:Az:699:UNK:HG2	35:Az:700:UNK:N	2.31	0.45
36:B0:126:LEU:HD13	36:B0:126:LEU:HA	1.82	0.45
40:B4:72:PRO:HG2	75:Bj:87:HIS:CG	2.52	0.45
46:BA:110:A:C5	46:BA:111:G:C8	3.05	0.45
46:BA:160:A:N6	46:BA:1034:A:N6	2.64	0.45
46:BA:177:C:H1'	61:BU:55:ARG:NH2	2.31	0.45
46:BA:218:A:OP1	77:Bl:91:MET:HG3	2.17	0.45
46:BA:521:U:H4'	46:BA:522:C:H5'	1.99	0.45
46:BA:576:A:N1	87:Bx:190:ARG:NH1	2.65	0.45
46:BA:717:C:O2'	66:Ba:112:ARG:HG3	2.16	0.45
46:BA:1388:G:H2'	46:BA:1389:U:C6	2.52	0.45
46:BA:1476:U:H2'	46:BA:1477:G:C8	2.49	0.45
48:BD:74:VAL:HG13	48:BD:151:TRP:NE1	2.31	0.45
54:BN:160:GLN:HA	54:BN:163:ILE:HD12	1.97	0.45
58:BR:46:TRP:CD1	58:BR:122:ALA:HB2	2.50	0.45
64:BX:10:TYR:HB3	70:Be:54:MET:HE3	1.99	0.45
66:Ba:337:GLU:H	66:Ba:337:GLU:CD	2.24	0.45
67:Bb:58:ARG:O	67:Bb:61:ALA:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:Bg:130:TRP:CH2	72:Bg:132:PRO:HA	2.51	0.45
73:Bh:105:ARG:CZ	73:Bh:113:GLU:HG3	2.46	0.45
75:Bj:216:LYS:HA	75:Bj:228:GLY:HA2	1.99	0.45
77:Bl:157:LEU:HD23	77:Bl:157:LEU:HA	1.71	0.45
84:Bu:165:UNK:HG2	84:Bu:165:UNK:O	2.17	0.45
88:Bz:417:UNK:HA	88:Bz:420:UNK:HG3	1.99	0.45
11:AN:115:ALA:HA	11:AN:120:LEU:HB2	1.98	0.45
15:AR:79:GLN:CD	22:Ad:190:ALA:HB2	2.41	0.45
16:AU:77:ARG:O	16:AU:80:ARG:NH1	2.50	0.45
19:Aa:124:ARG:HD3	33:Ap:169:GLN:HE22	1.81	0.45
23:Ae:200:UNK:HB1	23:Ae:226:UNK:CG	2.47	0.45
23:Ae:267:UNK:CG	33:Ap:218:ARG:HH11	2.30	0.45
23:Ae:354:UNK:HG1	23:Ae:357:UNK:HG3	1.90	0.45
25:Ag:382:LEU:HD13	25:Ag:393:LEU:HD22	1.98	0.45
32:Ao:160:UNK:CA	32:Ao:163:UNK:HG3	2.42	0.45
32:Ao:190:UNK:CG	32:Ao:223:UNK:HB2	2.47	0.45
34:As:2368:UNK:O	34:As:2371:UNK:HG3	2.16	0.45
40:B4:41:LEU:HD12	69:Bd:121:TRP:CH2	2.52	0.45
46:BA:128:A:C6	46:BA:129:A:C6	3.05	0.45
46:BA:204:A:O2'	46:BA:205:A:C8	2.67	0.45
46:BA:742:A:H4'	46:BA:742:A:OP1	2.16	0.45
46:BA:790:G:H2'	46:BA:791:A:C8	2.50	0.45
46:BA:1341:C:HO2'	46:BA:1386:A:HO2'	1.64	0.45
47:BB:38:P5P:H2'	47:BB:39:P5P:H8	1.98	0.45
52:BJ:100:GLN:NE2	81:Bp:34:LEU:HD23	2.32	0.45
56:BP:142:GLU:HB2	56:BP:162:LEU:HD23	1.98	0.45
59:BS:61:VAL:HG13	67:Bb:346:ARG:NH2	2.31	0.45
60:BT:244:ARG:HG2	60:BT:246:ASP:OD1	2.17	0.45
64:BX:69:ARG:HH12	86:Bw:266:PRO:HD3	1.77	0.45
72:Bg:29:LEU:HB3	72:Bg:31:PHE:HE1	1.82	0.45
74:Bi:173:VAL:O	74:Bi:176:ILE:HG22	2.17	0.45
74:Bi:179:LYS:HB3	74:Bi:225:TYR:O	2.17	0.45
74:Bi:205:GLN:HB2	74:Bi:207:ASN:HB2	1.99	0.45
77:Bl:127:PHE:CD2	77:Bl:128:LEU:HD13	2.52	0.45
83:Bt:57:GLU:HA	83:Bt:60:ARG:HG2	1.98	0.45
86:Bw:363:PHE:H	86:Bw:390:THR:HB	1.82	0.45
87:Bx:102:ARG:NE	87:Bx:107:LEU:O	2.40	0.45
88:Bz:9:UNK:HA	88:Bz:12:UNK:CG	2.46	0.45
1:AA:528:C:O2'	1:AA:928:A:N1	2.49	0.45
1:AA:532:G:H2'	1:AA:533:C:O4'	2.16	0.45
1:AA:647:A:C6	16:AU:82:ASP:HB3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:875:A:H61	28:Aj:17:ARG:HD3	1.80	0.45
7:AI:145:ARG:HA	7:AI:146:PRO:HD3	1.75	0.45
11:AN:62:ILE:HG21	26:Ah:341:HIS:HB3	1.98	0.45
12:AO:202:ARG:HB3	31:An:194:ILE:HG21	1.99	0.45
19:Aa:81:MET:HE3	19:Aa:287:GLN:HE22	1.82	0.45
23:Ae:200:UNK:HG1	23:Ae:226:UNK:CG	2.46	0.45
23:Ae:294:UNK:HG2	23:Ae:295:UNK:N	2.31	0.45
25:Ag:56:UNK:HB2	25:Ag:146:LYS:HZ2	1.80	0.45
25:Ag:83:PRO:HG3	25:Ag:135:LEU:HD13	1.98	0.45
31:An:174:LYS:HE2	31:An:178:GLN:HE22	1.82	0.45
46:BA:160:A:H5'	46:BA:161:G:C2	2.52	0.45
46:BA:288:U:H2'	46:BA:289:A:C8	2.52	0.45
46:BA:479:G:O2'	61:BU:98:ASN:OD1	2.23	0.45
46:BA:614:A:N3	79:Bn:41:ARG:NH2	2.64	0.45
46:BA:828:U:C4	46:BA:834:A:C4	3.05	0.45
46:BA:1268:G:C5	46:BA:1322:C:N3	2.84	0.45
47:BB:23:P5P:H8	47:BB:48:Y5P:H4	1.99	0.45
49:BE:222:TRP:CE2	49:BE:256:LYS:HB3	2.52	0.45
50:BF:166:PRO:HG2	50:BF:169:VAL:CG2	2.47	0.45
54:BN:112:LEU:HB3	54:BN:113:PRO:HD2	1.98	0.45
54:BN:171:SER:HB3	87:Bx:59:GLU:H	1.82	0.45
56:BP:61:THR:HG22	56:BP:61:THR:O	2.16	0.45
57:BQ:51:ARG:O	57:BQ:106:ARG:HD2	2.17	0.45
57:BQ:107:LEU:O	57:BQ:111:ARG:HG2	2.17	0.45
57:BQ:133:ARG:HD3	57:BQ:133:ARG:HA	1.72	0.45
62:BV:91:ILE:HD11	62:BV:145:PHE:CZ	2.51	0.45
63:BW:99:GLN:O	63:BW:102:ALA:HB3	2.17	0.45
63:BW:147:ARG:NH1	63:BW:150:TYR:CE1	2.85	0.45
64:BX:138:ASP:HB3	64:BX:141:ARG:HG2	1.99	0.45
65:BY:62:VAL:HG12	65:BY:122:LEU:HA	1.99	0.45
66:Ba:63:LYS:C	66:Ba:64:MET:HG3	2.41	0.45
66:Ba:110:ARG:HA	66:Ba:110:ARG:HD3	1.79	0.45
66:Ba:358:GLN:HE21	66:Ba:360:ASN:ND2	2.13	0.45
66:Ba:384:GLN:HB2	66:Ba:404:ILE:O	2.17	0.45
67:Bb:265:PHE:CE1	67:Bb:322:ARG:HD2	2.52	0.45
74:Bi:88:TYR:CD2	74:Bi:195:VAL:HG11	2.52	0.45
75:Bj:177:ASP:OD1	75:Bj:177:ASP:N	2.50	0.45
77:Bl:162:LEU:HD23	77:Bl:162:LEU:HA	1.63	0.45
84:Bu:185:GLU:O	84:Bu:189:LYS:HE3	2.17	0.45
88:Bz:29:UNK:CG	88:Bz:30:UNK:N	2.80	0.45
1:AA:155:A:H2'	1:AA:156:C:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:296:G:H4'	1:AA:297:A:H5"	1.98	0.44
1:AA:630:A:H2'	1:AA:631:A:C8	2.51	0.44
1:AA:937:A:H2'	1:AA:938:U:O4'	2.17	0.44
4:AE:203:LEU:HD11	4:AE:268:PHE:HB3	1.98	0.44
8:AJ:76:LEU:HD23	8:AJ:145:LEU:HD12	1.99	0.44
8:AJ:149:THR:HG21	29:Ak:133:THR:HG23	2.00	0.44
19:Aa:326:UNK:HA	19:Aa:329:UNK:CG	2.47	0.44
25:Ag:242:VAL:O	25:Ag:246:LEU:HB2	2.16	0.44
26:Ah:286:PHE:CE1	26:Ah:292:GLU:HA	2.52	0.44
29:Ak:141:SER:OG	29:Ak:144:LYS:HE3	2.16	0.44
36:B0:108:PRO:HD3	67:Bb:54:PHE:CZ	2.52	0.44
37:B1:77:LEU:HD12	37:B1:77:LEU:HA	1.77	0.44
46:BA:508:C:H42	46:BA:512:A:H3'	1.83	0.44
46:BA:1164:A:C2	46:BA:1170:A:N7	2.85	0.44
48:BD:74:VAL:HG22	48:BD:151:TRP:CD1	2.52	0.44
48:BD:127:VAL:HG12	48:BD:160:ALA:HA	1.98	0.44
50:BF:76:ARG:NH1	78:Bm:106:ALA:HB1	2.32	0.44
50:BF:87:PHE:O	50:BF:179:THR:HG23	2.17	0.44
60:BT:96:ARG:HH11	60:BT:285:GLU:CD	2.24	0.44
62:BV:88:ASN:ND2	62:BV:208:LEU:H	2.15	0.44
64:BX:66:ALA:N	64:BX:98:GLN:O	2.44	0.44
74:Bi:165:THR:HG21	74:Bi:262:HIS:ND1	2.32	0.44
88:Bz:13:UNK:C	88:Bz:16:UNK:HG3	2.43	0.44
88:Bz:610:UNK:CA	88:Bz:613:UNK:HG3	2.45	0.44
1:AA:180:U:O4	1:AA:181:A:N6	2.51	0.44
1:AA:503:A:HO2'	1:AA:504:C:P	2.38	0.44
4:AE:193:TRP:HZ2	4:AE:319:ALA:HA	1.82	0.44
6:AG:236:LEU:O	6:AG:239:TYR:HB2	2.17	0.44
8:AJ:75:ARG:H	8:AJ:175:THR:HG23	1.82	0.44
10:AL:69:LYS:HA	10:AL:70:PRO:HD3	1.67	0.44
19:Aa:220:GLN:HB2	19:Aa:222:GLN:CG	2.47	0.44
23:Ae:69:UNK:O	23:Ae:69:UNK:HG3	2.17	0.44
23:Ae:89:UNK:CG	60:BT:58:UNK:CG	2.96	0.44
23:Ae:120:UNK:CG	23:Ae:123:UNK:HG3	2.48	0.44
23:Ae:219:UNK:C	23:Ae:222:UNK:HG3	2.47	0.44
23:Ae:385:UNK:O	23:Ae:388:UNK:HG3	2.18	0.44
31:An:162:LEU:HA	31:An:165:LYS:HB2	1.99	0.44
32:Ao:203:UNK:CG	32:Ao:204:UNK:N	2.79	0.44
32:Ao:394:UNK:CA	32:Ao:397:UNK:HG3	2.44	0.44
32:Ao:420:UNK:HB2	32:Ao:459:UNK:CG	2.30	0.44
32:Ao:580:UNK:O	32:Ao:583:UNK:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Ap:88:GLN:HA	33:Ap:88:GLN:NE2	2.32	0.44
33:Ap:207:GLN:HA	33:Ap:208:PRO:HD3	1.74	0.44
36:B0:45:LYS:HB2	36:B0:45:LYS:HE3	1.77	0.44
36:B0:62:HIS:H	36:B0:65:ASN:ND2	2.15	0.44
38:B2:155:LEU:HD23	65:BY:193:THR:HG23	1.98	0.44
40:B4:41:LEU:HD12	69:Bd:121:TRP:HH2	1.83	0.44
44:B8:116:ARG:NH1	44:B8:167:LYS:HG2	2.32	0.44
46:BA:397:A:H2'	46:BA:398:A:H5'	1.98	0.44
46:BA:774:C:O2'	46:BA:775:A:H2'	2.17	0.44
46:BA:882:U:H2'	46:BA:883:G:O4'	2.17	0.44
46:BA:1343:A:C2	46:BA:1364:A:N6	2.83	0.44
48:BD:148:ARG:HE	48:BD:150:ARG:HG2	1.82	0.44
52:BJ:176:LEU:HB3	52:BJ:188:ARG:NH1	2.32	0.44
54:BN:152:PRO:HB3	87:Bx:84:GLU:HG3	1.98	0.44
56:BP:130:GLN:NE2	92:BP:402:HOH:O	2.23	0.44
56:BP:223:LEU:HD23	56:BP:223:LEU:HA	1.84	0.44
62:BV:167:LYS:HB2	72:Bg:106:ASP:HB3	1.99	0.44
64:BX:2:ALA:HA	64:BX:23:ASN:H	1.81	0.44
64:BX:75:GLY:N	64:BX:91:ASP:OD1	2.46	0.44
67:Bb:194:THR:HG22	67:Bb:196:THR:H	1.83	0.44
72:Bg:73:PRO:CB	72:Bg:89:ILE:HG13	2.47	0.44
73:Bh:227:GLU:OE1	73:Bh:302:ARG:NH1	2.50	0.44
74:Bi:80:CYS:HB2	74:Bi:166:GLU:HB2	2.00	0.44
75:Bj:152:LYS:HZ2	75:Bj:256:SER:CB	2.30	0.44
78:Bm:77:GLU:HG3	78:Bm:104:ARG:HH11	1.82	0.44
80:Bo:55:ARG:HA	80:Bo:56:PRO:HD3	1.88	0.44
88:Bz:610:UNK:O	88:Bz:613:UNK:HG3	2.17	0.44
1:AA:318:C:O2'	1:AA:319:A:OP2	2.34	0.44
1:AA:836:G:H2'	1:AA:837:C:H6	1.80	0.44
1:AA:931:G:H4'	1:AA:932:U:H5"	1.99	0.44
2:AB:168:ARG:HA	2:AB:168:ARG:HD3	1.58	0.44
3:AC:75:ASN:HD21	11:AN:104:TRP:NE1	2.15	0.44
4:AE:215:TYR:HB3	4:AE:218:PHE:CD2	2.53	0.44
9:AK:175:ILE:HA	16:AU:14:VAL:HG22	1.99	0.44
12:AO:158:LEU:HD12	12:AO:158:LEU:HA	1.81	0.44
21:Ac:162:LYS:HB3	21:Ac:162:LYS:HE2	1.70	0.44
23:Ae:284:UNK:O	23:Ae:288:UNK:HG3	2.17	0.44
23:Ae:359:UNK:O	23:Ae:362:UNK:CG	2.64	0.44
25:Ag:54:UNK:CG	25:Ag:67:UNK:HA	2.45	0.44
25:Ag:160:TRP:HE3	25:Ag:288:LEU:HB3	1.82	0.44
28:Aj:134:VAL:HB	28:Aj:135:MET:HE3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:Ao:317:UNK:HA	32:Ao:320:UNK:HG3	1.98	0.44
32:Ao:459:UNK:CA	32:Ao:462:UNK:HG3	2.48	0.44
38:B2:98:GLU:O	38:B2:101:HIS:HB3	2.17	0.44
39:B3:136:ASN:O	39:B3:149:TRP:HB2	2.17	0.44
41:B5:82:LYS:O	46:BA:1010:U:H4'	2.17	0.44
42:B6:36:ARG:NH1	46:BA:1184:U:OP1	2.50	0.44
46:BA:114:A:O2'	46:BA:115:U:H5"	2.17	0.44
46:BA:673:U:C5	64:BX:74:TYR:CD2	3.05	0.44
46:BA:691:U:H1'	46:BA:692:A:H5'	1.99	0.44
46:BA:1157:U:H1'	46:BA:1249:C:H2'	1.99	0.44
50:BF:227:PRO:HG2	50:BF:230:VAL:HG23	1.98	0.44
56:BP:202:LYS:HZ1	56:BP:296:SER:C	2.26	0.44
63:BW:147:ARG:CZ	63:BW:150:TYR:CE1	3.00	0.44
70:Be:126:PHE:HD2	70:Be:133:PHE:HB3	1.83	0.44
71:Bf:73:LYS:NZ	72:Bg:144:ARG:NH1	2.66	0.44
72:Bg:31:PHE:N	72:Bg:31:PHE:CD1	2.85	0.44
72:Bg:41:ARG:NH1	83:Bt:96:LEU:HB3	2.32	0.44
79:Bn:32:PHE:CD1	79:Bn:32:PHE:C	2.95	0.44
88:Bz:303:UNK:HA	88:Bz:306:UNK:HG3	1.99	0.44
1:AA:142:G:C2	1:AA:143:C:C2	3.05	0.44
1:AA:344:G:O2'	1:AA:437:C:H4'	2.18	0.44
1:AA:433:U:O2	1:AA:942:G:H4'	2.17	0.44
1:AA:672:A:H2'	1:AA:673:A:O4'	2.18	0.44
1:AA:822:A:H3'	1:AA:822:A:N3	2.32	0.44
4:AE:161:SER:OG	4:AE:164:ASP:HB2	2.16	0.44
8:AJ:164:LEU:HD21	8:AJ:170:MET:HB2	1.99	0.44
11:AN:64:PRO:HG2	11:AN:67:LEU:HB2	1.99	0.44
12:AO:129:ARG:HB2	12:AO:167:MET:HE1	1.99	0.44
13:AP:111:ARG:HG2	33:Ap:235:MET:HE1	1.98	0.44
17:AY:25:Y5P:O5'	17:AY:25:Y5P:H6	2.17	0.44
20:Ab:93:LYS:HB3	20:Ab:97:GLN:HG2	1.99	0.44
23:Ae:107:UNK:HA	23:Ae:110:UNK:HG3	2.00	0.44
23:Ae:131:UNK:O	23:Ae:136:UNK:N	2.50	0.44
23:Ae:174:UNK:HG3	23:Ae:177:UNK:HG3	1.98	0.44
28:Aj:142:VAL:HA	28:Aj:143:PRO:HD3	1.85	0.44
29:Ak:241:TRP:CD1	29:Ak:241:TRP:H	2.35	0.44
36:B0:90:TYR:CE1	36:B0:92:LEU:HD21	2.52	0.44
38:B2:80:LYS:NZ	74:Bi:71:ARG:NH2	2.64	0.44
40:B4:44:LEU:HD23	40:B4:46:ARG:H	1.83	0.44
46:BA:217:A:C2	67:Bb:379:ILE:HD13	2.53	0.44
46:BA:1232:U:H3'	46:BA:1233:C:H6	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:BF:190:VAL:HG13	50:BF:191:ASP:O	2.18	0.44
51:BI:105:LEU:HD22	51:BI:112:VAL:HG21	2.00	0.44
52:BJ:34:THR:OG1	52:BJ:35:ARG:N	2.49	0.44
56:BP:237:ALA:O	56:BP:241:GLY:N	2.50	0.44
60:BT:99:MET:HB3	60:BT:145:LEU:HD12	2.00	0.44
67:Bb:292:GLN:HB2	67:Bb:295:GLN:CD	2.42	0.44
68:Bc:102:LEU:HA	68:Bc:102:LEU:HD12	1.74	0.44
75:Bj:162:ARG:HB3	75:Bj:251:HIS:CD2	2.53	0.44
1:AA:232:G:H5"	4:AE:196:ASN:HD22	1.83	0.44
1:AA:687:A:C4	11:AN:109:ILE:HG21	2.53	0.44
2:AB:142:LEU:HA	2:AB:164:TYR:O	2.17	0.44
3:AC:85:ARG:CZ	29:Ak:163:PRO:HD2	2.48	0.44
6:AG:119:LYS:NZ	25:Ag:397:LEU:C	2.76	0.44
6:AG:190:GLU:O	6:AG:194:LYS:HG2	2.18	0.44
6:AG:204:LYS:O	6:AG:208:GLU:HG2	2.17	0.44
6:AG:231:GLU:OE2	30:Am:57:LYS:HE3	2.16	0.44
9:AK:131:GLN:HB2	9:AK:169:MET:HE1	1.99	0.44
13:AP:101:PRO:O	13:AP:105:THR:OG1	2.26	0.44
14:AQ:33:LEU:HB2	21:Ac:56:GLN:HE21	1.82	0.44
19:Aa:118:VAL:O	19:Aa:122:LYS:HG2	2.18	0.44
25:Ag:52:UNK:HG1	25:Ag:66:UNK:N	2.32	0.44
25:Ag:57:UNK:CG	25:Ag:142:HIS:CE1	3.00	0.44
27:Ai:14:LEU:O	27:Ai:18:LEU:HB2	2.17	0.44
37:B1:155:SER:HB2	37:B1:158:GLY:H	1.82	0.44
37:B1:173:ASP:HA	37:B1:174:PRO:HD3	1.80	0.44
39:B3:65:LYS:HE2	80:Bo:84:MET:HE3	2.00	0.44
44:B8:95:THR:HB	44:B8:105:LYS:HB2	1.99	0.44
44:B8:142:ARG:CZ	44:B8:142:ARG:HB2	2.46	0.44
44:B8:172:TYR:CE1	56:BP:90:ARG:NH1	2.86	0.44
46:BA:777:G:H5'	46:BA:778:G:OP2	2.18	0.44
46:BA:1178:G:C2	46:BA:1179:A:C8	3.06	0.44
53:BK:60:ILE:HG21	53:BK:64:ILE:HG13	1.99	0.44
60:BT:229:TRP:HH2	60:BT:249:LEU:HD21	1.83	0.44
62:BV:137:VAL:HG12	62:BV:153:LEU:HD23	1.99	0.44
63:BW:49:TRP:HD1	63:BW:74:CYS:HG	1.66	0.44
63:BW:76:ARG:CA	63:BW:171:HIS:HD2	2.28	0.44
71:Bf:79:UNK:O	71:Bf:79:UNK:CG	2.64	0.44
72:Bg:139:THR:OG1	72:Bg:140:LEU:N	2.50	0.44
74:Bi:168:CYS:HB2	74:Bi:262:HIS:O	2.17	0.44
74:Bi:245:TYR:CD1	74:Bi:265:ILE:HB	2.48	0.44
77:Bl:122:LYS:HA	77:Bl:122:LYS:HD3	1.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:Bw:329:TRP:O	86:Bw:333:GLN:HG3	2.17	0.44
1:AA:85:G:H2'	1:AA:86:A:C8	2.53	0.44
2:AB:114:ILE:HD13	24:Af:85:LEU:HD11	1.99	0.44
2:AB:233:TYR:OH	20:Ab:40:PRO:HD3	2.17	0.44
4:AE:321:MET:HE2	4:AE:321:MET:HB3	1.89	0.44
5:AF:92:ASN:OD1	15:AR:118:LEU:HD22	2.16	0.44
6:AG:98:MET:HE2	6:AG:98:MET:HB3	1.74	0.44
13:AP:110:LEU:O	13:AP:114:ARG:HG2	2.16	0.44
23:Ae:98:UNK:HG2	23:Ae:100:UNK:HG2	2.00	0.44
23:Ae:98:UNK:HG2	23:Ae:100:UNK:HG3	1.99	0.44
23:Ae:98:UNK:CG	23:Ae:100:UNK:CG	2.96	0.44
24:Af:173:LEU:HD23	24:Af:173:LEU:H	1.82	0.44
25:Ag:52:UNK:CG	25:Ag:66:UNK:N	2.80	0.44
28:Aj:83:LYS:HE2	28:Aj:87:TRP:CZ2	2.52	0.44
29:Ak:170:ALA:O	29:Ak:217:LYS:HE2	2.17	0.44
30:Am:44:THR:O	30:Am:45:CYS:HB2	2.18	0.44
32:Ao:396:UNK:HA	32:Ao:399:UNK:HG3	2.00	0.44
36:B0:51:PHE:HA	36:B0:69:THR:HG23	1.99	0.44
36:B0:76:HIS:CD2	59:BS:70:THR:HG21	2.52	0.44
39:B3:81:TRP:CD1	39:B3:82:GLU:N	2.86	0.44
46:BA:108:A:C2	46:BA:131:G:C8	3.05	0.44
46:BA:163:A:P	61:BU:52:LYS:NZ	2.90	0.44
46:BA:346:U:O4'	46:BA:348:A:H5'	2.17	0.44
46:BA:838:C:H2'	46:BA:839:A:O4'	2.18	0.44
47:BB:24:P5P:H4'	59:BS:108:ARG:HD2	2.00	0.44
47:BB:32:P5P:C5	47:BB:33:Y5P:H4	2.48	0.44
50:BF:105:ASN:O	50:BF:107:LYS:N	2.50	0.44
50:BF:192:SER:O	50:BF:193:LEU:HB2	2.18	0.44
53:BK:111:LEU:HD11	53:BK:154:ARG:HE	1.82	0.44
54:BN:169:VAL:HG13	87:Bx:75:TRP:CD1	2.53	0.44
56:BP:51:ARG:HB3	56:BP:51:ARG:HH11	1.82	0.44
56:BP:244:LEU:HD12	56:BP:245:PRO:HD2	1.99	0.44
58:BR:15:PHE:HB3	58:BR:25:ARG:HH12	1.82	0.44
64:BX:141:ARG:HH11	74:Bi:276:ILE:HD11	1.80	0.44
66:Ba:302:ARG:HD3	66:Ba:302:ARG:HA	1.60	0.44
68:Bc:259:ASP:OD1	68:Bc:260:VAL:N	2.51	0.44
71:Bf:89:UNK:O	71:Bf:92:UNK:HG3	2.18	0.44
77:Bl:140:VAL:H	83:Bt:85:HIS:HD2	1.58	0.44
86:Bw:245:VAL:HG22	86:Bw:388:TRP:HH2	1.82	0.44
1:AA:202:A:H5'	13:AP:102:MET:CE	2.48	0.44
1:AA:333:A:N7	1:AA:361:A:H2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:557:G:C2	1:AA:558:U:C2	3.06	0.44
1:AA:794:A:OP1	7:AI:390:ARG:NH1	2.50	0.44
4:AE:128:ARG:HD3	4:AE:179:TRP:CZ2	2.53	0.44
13:AP:65:LEU:HB3	19:Aa:195:TYR:OH	2.17	0.44
19:Aa:344:UNK:CA	19:Aa:347:UNK:HG3	2.47	0.44
25:Ag:137:LEU:HD11	25:Ag:260:ALA:HB1	2.00	0.44
25:Ag:252:LEU:HB2	25:Ag:254:ILE:HG12	1.99	0.44
39:B3:67:HIS:NE2	39:B3:102:ASN:OD1	2.49	0.44
40:B4:35:ASP:HB3	76:Bk:177:ASN:ND2	2.31	0.44
43:B7:95:HIS:CD2	70:Be:17:ARG:HE	2.36	0.44
45:B9:63:PHE:N	46:BA:1347:G:N3	2.66	0.44
46:BA:205:A:O2'	46:BA:236:A:N7	2.41	0.44
46:BA:230:C:H6	46:BA:230:C:OP2	1.99	0.44
46:BA:774:C:O2'	46:BA:775:A:O5'	2.30	0.44
53:BK:23:ILE:HA	53:BK:67:PRO:HA	2.00	0.44
56:BP:142:GLU:HB3	56:BP:162:LEU:HB3	2.00	0.44
57:BQ:213:TRP:CZ3	57:BQ:217:ARG:NH1	2.85	0.44
60:BT:54:UNK:O	60:BT:54:UNK:HG2	2.18	0.44
65:BY:159:PHE:CD1	65:BY:160:PRO:HD2	2.53	0.44
66:Ba:309:LEU:HD23	66:Ba:353:GLN:HG3	2.00	0.44
67:Bb:158:TYR:HE1	67:Bb:167:PHE:H	1.66	0.44
74:Bi:231:LEU:HD12	74:Bi:232:MET:H	1.82	0.44
78:Bm:90:ILE:O	78:Bm:124:VAL:HG23	2.18	0.44
78:Bm:139:SER:OG	78:Bm:140:LYS:N	2.50	0.44
84:Bu:103:HIS:HD2	84:Bu:106:SER:N	2.15	0.44
86:Bw:118:LEU:CG	86:Bw:119:PRO:HD2	2.45	0.44
86:Bw:313:GLN:O	86:Bw:317:VAL:HG23	2.17	0.44
87:Bx:181:LEU:HD23	87:Bx:181:LEU:HA	1.68	0.44
88:Bz:604:UNK:HA	88:Bz:607:UNK:HG3	2.00	0.44
1:AA:25:U:H2'	1:AA:26:A:C8	2.52	0.44
2:AB:241:SER:HA	2:AB:242:PRO:HD3	1.85	0.44
3:AC:101:PRO:HB3	27:Ai:72:ARG:HD3	1.99	0.44
7:AI:294:ILE:HG23	7:AI:301:TYR:CD1	2.53	0.44
9:AK:141:ALA:O	9:AK:146:VAL:HG22	2.17	0.44
13:AP:77:ILE:HD11	13:AP:83:LEU:HD11	2.00	0.44
19:Aa:344:UNK:HA	19:Aa:347:UNK:CG	2.47	0.44
23:Ae:243:UNK:C	23:Ae:244:UNK:CG	2.96	0.44
23:Ae:253:UNK:HA	23:Ae:256:UNK:HG3	1.99	0.44
23:Ae:258:UNK:HA	23:Ae:261:UNK:HG3	2.00	0.44
25:Ag:64:UNK:HG1	25:Ag:350:LYS:HD2	2.00	0.44
30:Am:46:ILE:O	30:Am:49:MET:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:B2:144:LEU:O	38:B2:148:VAL:HG23	2.17	0.44
39:B3:73:LYS:HE2	39:B3:73:LYS:HB3	1.66	0.44
40:B4:42:THR:O	40:B4:68:ARG:NH1	2.48	0.44
46:BA:13:U:C2	46:BA:105:G:C2	3.06	0.44
46:BA:214:A:H2'	46:BA:215:C:O4'	2.17	0.44
46:BA:724:A:H4'	46:BA:725:A:OP1	2.18	0.44
46:BA:801:A:H61	46:BA:809:A:H61	1.64	0.44
46:BA:1557:A:H4'	49:BE:263:ASN:HD21	1.83	0.44
48:BD:154:ALA:O	48:BD:249:SER:OG	2.35	0.44
49:BE:235:LYS:O	49:BE:239:ARG:HD2	2.18	0.44
50:BF:262:THR:O	50:BF:265:THR:HB	2.18	0.44
56:BP:54:LYS:HB3	56:BP:55:GLY:H	1.45	0.44
59:BS:81:LEU:HD12	59:BS:93:LEU:O	2.17	0.44
59:BS:114:LYS:HE2	67:Bb:138:GLU:HG3	1.99	0.44
59:BS:130:ARG:NH1	67:Bb:129:ARG:NH1	2.65	0.44
60:BT:234:GLU:H	60:BT:234:GLU:HG2	1.42	0.44
67:Bb:337:MET:HE2	67:Bb:337:MET:HB3	1.60	0.44
69:Bd:120:ARG:CZ	75:Bj:66:LEU:HD13	2.47	0.44
72:Bg:89:ILE:H	72:Bg:89:ILE:HG12	1.54	0.44
73:Bh:258:THR:HG22	73:Bh:259:ARG:HG2	2.00	0.44
73:Bh:270:TYR:O	73:Bh:285:PRO:HA	2.17	0.44
78:Bm:113:VAL:HG22	78:Bm:130:PHE:CE2	2.52	0.44
86:Bw:306:LEU:HD23	86:Bw:306:LEU:HA	1.80	0.44
88:Bz:24:UNK:HA	88:Bz:27:UNK:CG	2.48	0.44
2:AB:168:ARG:HG2	7:AI:159:TYR:CZ	2.53	0.44
4:AE:124:LYS:HD3	27:Ai:81:GLU:OE2	2.18	0.44
4:AE:305:MET:HE2	4:AE:332:LEU:HD21	2.00	0.44
5:AF:50:LYS:HD2	5:AF:57:ARG:NH2	2.33	0.44
7:AI:158:TYR:OH	7:AI:218:ASP:O	2.34	0.44
7:AI:161:LEU:O	7:AI:165:THR:OG1	2.19	0.44
9:AK:194:ARG:O	9:AK:195:ARG:NH1	2.51	0.44
22:Ad:68:ARG:HH11	28:Aj:198:ILE:HG12	1.83	0.44
23:Ae:169:UNK:O	23:Ae:170:UNK:HG3	2.18	0.44
23:Ae:296:UNK:O	23:Ae:299:UNK:HG3	2.18	0.44
25:Ag:155:PRO:O	25:Ag:262:ASP:HB3	2.17	0.44
29:Ak:148:HIS:O	29:Ak:150:PRO:HD3	2.18	0.44
32:Ao:461:UNK:HA	32:Ao:464:UNK:HG3	2.00	0.44
32:Ao:486:UNK:O	32:Ao:486:UNK:CG	2.65	0.44
33:Ap:213:LEU:O	33:Ap:217:ARG:HG3	2.17	0.44
41:B5:95:ARG:HH11	46:BA:156:A:H5'	1.83	0.44
46:BA:222:A:O2'	46:BA:223:A:C8	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:BA:356:U:H5'	46:BA:357:U:P	2.58	0.44
46:BA:1037:A:H2'	46:BA:1038:A:O4'	2.17	0.44
46:BA:1192:U:H2'	46:BA:1193:A:H5"	2.00	0.44
92:BA:1912:HOH:O	56:BP:130:GLN:NE2	2.51	0.44
50:BF:211:ARG:HB2	78:Bm:59:ARG:NH2	2.32	0.44
52:BJ:161:VAL:HB	52:BJ:195:SER:HA	1.99	0.44
53:BK:137:LEU:HD12	53:BK:137:LEU:HA	1.82	0.44
56:BP:100:ARG:HH11	56:BP:100:ARG:HG3	1.82	0.44
57:BQ:211:ASN:HA	57:BQ:212:PRO:HD3	1.67	0.44
60:BT:100:LEU:HD23	60:BT:100:LEU:HA	1.78	0.44
64:BX:148:PHE:CD1	74:Bi:222:LEU:HD22	2.53	0.44
66:Ba:165:HIS:HD2	86:Bw:198:ARG:HD3	1.82	0.44
68:Bc:240:LYS:HA	68:Bc:240:LYS:HD2	1.59	0.44
68:Bc:282:ASN:HD21	68:Bc:291:ARG:NH1	2.16	0.44
78:Bm:125:ARG:HA	78:Bm:128:LEU:HD12	1.99	0.44
86:Bw:88:PHE:HA	86:Bw:271:GLN:NE2	2.33	0.44
86:Bw:166:ILE:HA	86:Bw:166:ILE:HD13	1.82	0.44
86:Bw:199:PRO:HA	86:Bw:229:ASP:O	2.18	0.44
86:Bw:397:GLU:HB2	86:Bw:406:GLY:HA3	1.99	0.44
3:AC:92:LEU:HA	3:AC:92:LEU:HD23	1.74	0.43
19:Aa:249:TYR:HA	19:Aa:252:ILE:HG12	2.00	0.43
23:Ae:362:UNK:HG2	23:Ae:363:UNK:N	2.32	0.43
24:Af:98:ASN:ND2	24:Af:144:ARG:HH21	2.16	0.43
28:Aj:31:SER:HA	28:Aj:111:HIS:CD2	2.53	0.43
32:Ao:189:UNK:C	32:Ao:192:UNK:HG3	2.48	0.43
32:Ao:652:UNK:HB2	32:Ao:674:UNK:O	2.18	0.43
33:Ap:192:THR:HG21	33:Ap:199:TRP:HA	2.00	0.43
33:Ap:217:ARG:HG2	33:Ap:224:LEU:HD21	2.00	0.43
37:B1:216:ARG:HD3	37:B1:217:LEU:HD23	2.00	0.43
40:B4:79:PRO:HG2	88:Bz:106:UNK:HB2	2.00	0.43
44:B8:97:PHE:H	79:Bn:122:ASN:HD21	1.66	0.43
44:B8:148:VAL:HG12	67:Bb:361:GLN:N	2.33	0.43
44:B8:183:ARG:HH12	67:Bb:354:GLN:HE21	1.64	0.43
46:BA:30:U:H5'	46:BA:31:A:OP1	2.18	0.43
46:BA:64:C:N3	46:BA:65:C:C4	2.86	0.43
46:BA:160:A:H62	46:BA:1034:A:H62	1.66	0.43
46:BA:197:U:H2'	46:BA:198:A:C8	2.53	0.43
46:BA:378:U:H1'	56:BP:68:GLU:OE1	2.18	0.43
46:BA:462:A:H3'	46:BA:463:U:C5'	2.47	0.43
46:BA:812:C:O2	46:BA:812:C:H2'	2.17	0.43
46:BA:1340:C:C5	46:BA:1362:A:C6	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:BE:165:TYR:CD2	49:BE:172:PRO:HA	2.53	0.43
50:BF:63:GLN:HE21	50:BF:81:GLU:HG3	1.83	0.43
50:BF:95:ILE:H	50:BF:95:ILE:HG13	1.51	0.43
56:BP:53:HIS:CD2	56:BP:53:HIS:C	2.94	0.43
59:BS:122:VAL:HB	67:Bb:126:GLN:OE1	2.18	0.43
67:Bb:324:ASP:OD1	67:Bb:326:SER:OG	2.35	0.43
72:Bg:53:ASP:HB3	72:Bg:57:ARG:HH21	1.82	0.43
77:Bl:60:PRO:HA	77:Bl:61:PRO:HD3	1.87	0.43
82:Bq:122:ARG:O	82:Bq:126:ILE:HG12	2.19	0.43
84:Bu:103:HIS:HD2	84:Bu:106:SER:H	1.64	0.43
86:Bw:267:LEU:HD22	86:Bw:268:PHE:H	1.82	0.43
87:Bx:171:LYS:HD2	87:Bx:171:LYS:HA	1.79	0.43
88:Bz:414:UNK:C	88:Bz:417:UNK:HG3	2.48	0.43
1:AA:386:U:H2'	1:AA:387:C:C6	2.54	0.43
1:AA:476:A:C8	30:Am:13:LEU:HD23	2.53	0.43
7:AI:376:ARG:NH1	7:AI:376:ARG:HG3	2.33	0.43
20:Ab:11:SER:O	20:Ab:14:SER:OG	2.33	0.43
22:Ad:52:GLU:O	22:Ad:56:LEU:HG	2.18	0.43
23:Ae:161:UNK:O	23:Ae:165:UNK:HB2	2.17	0.43
23:Ae:215:UNK:O	23:Ae:219:UNK:HG3	2.17	0.43
23:Ae:218:UNK:O	23:Ae:221:UNK:HG3	2.18	0.43
25:Ag:365:LEU:HD12	25:Ag:365:LEU:HA	1.75	0.43
26:Ah:371:TYR:CZ	26:Ah:375:LYS:NZ	2.83	0.43
38:B2:175:PHE:CZ	43:B7:82:ILE:HG21	2.53	0.43
42:B6:47:ASP:HA	42:B6:48:PRO:HD3	1.68	0.43
46:BA:980:U:O2	46:BA:980:U:H2'	2.17	0.43
46:BA:1030:G:H2'	46:BA:1031:G:H8	1.83	0.43
52:BJ:117:ARG:HD3	52:BJ:117:ARG:HA	1.75	0.43
55:BO:69:VAL:CG1	55:BO:127:LEU:HD21	2.48	0.43
56:BP:83:PHE:HD1	56:BP:83:PHE:HA	1.66	0.43
60:BT:74:ARG:HB3	60:BT:283:TRP:CH2	2.53	0.43
66:Ba:281:GLU:O	86:Bw:150:PHE:HE1	2.01	0.43
67:Bb:189:HIS:HA	67:Bb:318:PHE:H	1.83	0.43
74:Bi:90:PRO:HB2	74:Bi:269:TRP:CH2	2.47	0.43
79:Bn:89:GLN:HA	79:Bn:92:ILE:HG22	2.00	0.43
86:Bw:414:GLN:O	86:Bw:417:GLN:HB2	2.17	0.43
1:AA:59:C:OP1	28:Aj:51:PRO:HG3	2.19	0.43
1:AA:127:A:C2	1:AA:128:C:C4	3.06	0.43
1:AA:612:U:H5'	1:AA:613:A:OP2	2.18	0.43
1:AA:761:U:H2'	1:AA:762:G:O4'	2.17	0.43
3:AC:133:TYR:OH	32:Ao:90:GLN:N	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AE:370:VAL:HG12	19:Aa:104:LEU:HD23	1.99	0.43
7:AI:309:GLN:HG2	7:AI:313:GLN:HE21	1.82	0.43
7:AI:331:CYS:SG	7:AI:332:ALA:N	2.91	0.43
19:Aa:160:ILE:O	19:Aa:160:ILE:HG12	2.19	0.43
19:Aa:193:GLN:HG3	19:Aa:203:ILE:HG12	1.99	0.43
19:Aa:216:THR:O	19:Aa:220:GLN:HG2	2.19	0.43
21:Ac:75:PHE:HA	21:Ac:90:VAL:HG22	2.01	0.43
23:Ae:73:UNK:CG	23:Ae:74:UNK:N	2.81	0.43
23:Ae:301:UNK:CA	23:Ae:304:UNK:HG3	2.40	0.43
23:Ae:390:UNK:HA	23:Ae:393:UNK:CG	2.46	0.43
23:Ae:393:UNK:HA	23:Ae:396:UNK:HG3	1.99	0.43
23:Ae:398:UNK:O	23:Ae:401:UNK:HG3	2.18	0.43
24:Af:160:ASP:OD1	24:Af:160:ASP:N	2.51	0.43
25:Ag:102:LYS:N	25:Ag:103:PRO:HD2	2.34	0.43
28:Aj:98:THR:HG22	28:Aj:99:ARG:HG3	1.99	0.43
30:Am:52:MET:HE3	30:Am:53:MET:HE3	2.01	0.43
30:Am:84:ARG:HG2	30:Am:87:ARG:HH12	1.80	0.43
32:Ao:190:UNK:O	32:Ao:193:UNK:HG3	2.19	0.43
32:Ao:320:UNK:C	32:Ao:323:UNK:HG3	2.47	0.43
32:Ao:501:UNK:O	32:Ao:505:UNK:HG3	2.18	0.43
32:Ao:655:UNK:HA	32:Ao:658:UNK:HG3	2.00	0.43
32:Ao:656:UNK:CA	32:Ao:674:UNK:HG1	2.49	0.43
36:B0:102:GLU:OE2	67:Bb:74:TYR:HB2	2.18	0.43
38:B2:115:LEU:O	38:B2:118:GLU:HB3	2.18	0.43
46:BA:63:A:C5	79:Bn:118:TYR:CE2	3.06	0.43
46:BA:196:U:H2'	46:BA:197:U:C6	2.53	0.43
46:BA:217:A:H4'	46:BA:218:A:H5'	2.00	0.43
46:BA:697:G:H2'	46:BA:698:A:C8	2.53	0.43
46:BA:699:U:H2'	46:BA:700:A:O4'	2.18	0.43
49:BE:208:ALA:HB3	49:BE:290:PRO:O	2.18	0.43
50:BF:63:GLN:HA	50:BF:80:THR:O	2.18	0.43
50:BF:107:LYS:HA	79:Bn:74:ILE:CD1	2.48	0.43
50:BF:205:GLU:CG	50:BF:208:ARG:HH12	2.24	0.43
50:BF:250:VAL:HA	50:BF:253:MET:HE3	1.99	0.43
58:BR:13:ARG:HH11	58:BR:13:ARG:HG3	1.84	0.43
59:BS:178:ILE:HG22	59:BS:179:TYR:HD1	1.84	0.43
63:BW:150:TYR:HE2	63:BW:168:VAL:HG13	1.83	0.43
65:BY:196:GLU:O	65:BY:200:GLU:HB3	2.17	0.43
66:Ba:125:LYS:HE3	66:Ba:364:LEU:HA	1.99	0.43
67:Bb:198:ALA:HB1	67:Bb:257:PRO:HD2	1.99	0.43
67:Bb:326:SER:O	67:Bb:329:ARG:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:Bc:181:VAL:HG13	68:Bc:289:LEU:O	2.18	0.43
68:Bc:207:ILE:HA	68:Bc:269:THR:HG22	2.00	0.43
74:Bi:221:THR:HG22	74:Bi:239:PRO:HA	2.00	0.43
75:Bj:191:THR:HG23	75:Bj:195:LEU:HD13	1.99	0.43
77:Bl:106:GLN:C	77:Bl:107:MET:HG3	2.44	0.43
78:Bm:71:LEU:HD13	78:Bm:128:LEU:HD23	1.99	0.43
86:Bw:51:LEU:HD22	86:Bw:51:LEU:HA	1.75	0.43
86:Bw:241:LEU:HD11	86:Bw:290:HIS:CE1	2.52	0.43
86:Bw:267:LEU:HD23	86:Bw:267:LEU:HA	1.54	0.43
1:AA:48:C:N4	1:AA:172:A:OP2	2.46	0.43
1:AA:835:C:H2'	1:AA:836:G:H8	1.77	0.43
1:AA:938:U:H2'	1:AA:939:A:C8	2.53	0.43
2:AB:117:LEU:HD12	24:Af:81:PHE:CE1	2.54	0.43
6:AG:68:PHE:HB3	7:AI:367:GLN:NE2	2.33	0.43
23:Ae:35:UNK:O	23:Ae:38:UNK:HG3	2.18	0.43
23:Ae:71:UNK:O	23:Ae:75:UNK:HB1	2.18	0.43
23:Ae:79:UNK:HG1	23:Ae:88:UNK:CB	2.48	0.43
24:Af:154:PHE:HB3	30:Am:29:LEU:HD22	2.00	0.43
25:Ag:57:UNK:HB2	25:Ag:143:PHE:HD1	1.83	0.43
36:B0:74:ARG:HG3	46:BA:401:A:O4'	2.18	0.43
39:B3:51:GLU:CD	39:B3:51:GLU:H	2.26	0.43
44:B8:163:THR:HG21	46:BA:76:G:H5"	1.99	0.43
46:BA:82:G:H5'	46:BA:83:A:H5'	2.00	0.43
46:BA:228:A:H2'	77:Bl:98:ARG:O	2.18	0.43
46:BA:857:A:H5"	48:BD:67:LYS:HE2	1.99	0.43
46:BA:899:C:C5	46:BA:923:G:C6	3.05	0.43
46:BA:1230:G:H5"	46:BA:1230:G:C8	2.51	0.43
47:BB:61:Y5P:H2'	47:BB:62:Y5P:H6	1.99	0.43
48:BD:198:GLU:HA	48:BD:205:ALA:HA	2.01	0.43
49:BE:296:LEU:HA	49:BE:296:LEU:HD12	1.61	0.43
52:BJ:49:ALA:HB1	83:Bt:32:LYS:HE2	2.01	0.43
52:BJ:163:GLU:N	52:BJ:163:GLU:OE1	2.52	0.43
59:BS:52:ASN:OD1	59:BS:55:ASN:HB2	2.18	0.43
62:BV:180:LYS:O	62:BV:182:LYS:HG2	2.18	0.43
65:BY:183:LEU:HD21	70:Be:77:PRO:HD2	2.01	0.43
66:Ba:380:GLN:HB3	66:Ba:410:THR:HG22	1.99	0.43
69:Bd:168:LEU:HD23	69:Bd:168:LEU:HA	1.82	0.43
71:Bf:116:PHE:CD1	73:Bh:267:LEU:HD21	2.54	0.43
74:Bi:179:LYS:HD3	74:Bi:232:MET:HE1	2.00	0.43
77:Bl:147:LEU:HD12	77:Bl:147:LEU:HA	1.76	0.43
87:Bx:93:ILE:HG22	87:Bx:98:GLY:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AE:260:LYS:HB3	4:AE:260:LYS:HE2	1.70	0.43
6:AG:45:GLN:HB3	6:AG:51:TYR:OH	2.18	0.43
13:AP:111:ARG:HG2	33:Ap:235:MET:SD	2.59	0.43
16:AU:50:ARG:HH11	16:AU:50:ARG:CG	2.32	0.43
20:Ab:103:TYR:CE1	20:Ab:117:LEU:HD13	2.53	0.43
22:Ad:62:GLN:O	22:Ad:65:GLN:HB3	2.18	0.43
23:Ae:92:UNK:CG	23:Ae:93:UNK:N	2.79	0.43
32:Ao:221:UNK:HG2	32:Ao:222:UNK:N	2.33	0.43
32:Ao:270:UNK:HA	32:Ao:273:UNK:HG3	2.00	0.43
32:Ao:359:UNK:HG1	32:Ao:396:UNK:HG1	1.95	0.43
32:Ao:422:UNK:O	32:Ao:426:UNK:HB1	2.18	0.43
32:Ao:504:UNK:HB2	32:Ao:537:UNK:HB2	2.00	0.43
33:Ap:54:GLU:HA	33:Ap:55:PRO:HD3	1.63	0.43
38:B2:192:LEU:HD23	38:B2:192:LEU:HA	1.81	0.43
46:BA:162:C:O2	46:BA:162:C:H2'	2.18	0.43
46:BA:397:A:C5	46:BA:398:A:C8	3.06	0.43
46:BA:537:U:O4	46:BA:538:A:N6	2.51	0.43
46:BA:1228:U:H5'	46:BA:1229:U:O5'	2.18	0.43
56:BP:282:ILE:HG13	77:Bl:44:GLU:HB2	2.01	0.43
57:BQ:88:ALA:HA	57:BQ:161:VAL:O	2.17	0.43
65:BY:73:GLN:CD	65:BY:123:VAL:HG21	2.43	0.43
66:Ba:44:PRO:HG2	66:Ba:72:ARG:NH2	2.34	0.43
66:Ba:240:ALA:HB2	66:Ba:375:TRP:HH2	1.83	0.43
67:Bb:175:VAL:HG11	67:Bb:270:PHE:CZ	2.54	0.43
68:Bc:61:LYS:HD3	68:Bc:61:LYS:HA	1.74	0.43
68:Bc:282:ASN:ND2	68:Bc:291:ARG:HD3	2.33	0.43
71:Bf:52:THR:HG22	71:Bf:54:ASP:H	1.83	0.43
72:Bg:144:ARG:HH22	73:Bh:260:GLN:HE22	1.66	0.43
88:Bz:22:UNK:HG2	88:Bz:23:UNK:N	2.33	0.43
1:AA:670:A:H2'	1:AA:671:U:C6	2.53	0.43
1:AA:792:U:H4'	7:AI:389:ARG:HG3	2.00	0.43
7:AI:131:ILE:HD13	29:Ak:88:ARG:HD2	2.00	0.43
8:AJ:163:ASN:HB3	29:Ak:116:LEU:HD11	1.99	0.43
8:AJ:179:GLN:H	8:AJ:179:GLN:HG2	1.59	0.43
12:AO:68:PRO:HG2	12:AO:108:LYS:HE3	1.99	0.43
13:AP:86:PRO:HA	13:AP:89:LYS:HG2	2.01	0.43
13:AP:111:ARG:NH1	19:Aa:146:ILE:HG22	2.33	0.43
15:AR:112:ILE:HG23	15:AR:121:MET:HE1	2.00	0.43
16:AU:13:MET:HE2	16:AU:13:MET:HB3	1.94	0.43
17:AV:51:Y5P:H2'	17:AV:52:Y5P:H6	1.98	0.43
23:Ae:84:UNK:HG1	23:Ae:86:UNK:HG3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Ae:399:UNK:O	23:Ae:402:UNK:CG	2.65	0.43
27:Ai:31:MET:HE3	27:Ai:34:VAL:HG21	2.00	0.43
28:Aj:65:LEU:HD21	28:Aj:102:PRO:HB3	2.01	0.43
29:Ak:286:LEU:HD23	29:Ak:291:VAL:HG11	2.01	0.43
32:Ao:228:UNK:HB2	32:Ao:244:UNK:HG1	2.00	0.43
36:B0:92:LEU:C	36:B0:93:GLU:HG2	2.44	0.43
37:B1:118:ILE:O	37:B1:168:ARG:HD3	2.18	0.43
40:B4:73:ARG:NH2	40:B4:76:LEU:HD13	2.32	0.43
43:B7:85:ARG:NH1	43:B7:90:ARG:HD2	2.33	0.43
46:BA:112:A:C2	46:BA:114:A:C6	3.06	0.43
46:BA:217:A:C5	67:Bb:379:ILE:HG21	2.52	0.43
46:BA:242:A:C6	46:BA:243:A:C6	3.06	0.43
46:BA:355:G:N2	46:BA:356:U:H1'	2.34	0.43
46:BA:654:C:O2	46:BA:655:U:N3	2.42	0.43
50:BF:92:ARG:HG2	50:BF:95:ILE:HG13	2.01	0.43
54:BN:140:ASN:HB2	73:Bh:262:GLY:HA2	1.94	0.43
56:BP:56:GLU:OE2	56:BP:61:THR:HB	2.17	0.43
56:BP:247:ILE:H	56:BP:247:ILE:HD12	1.83	0.43
59:BS:88:HIS:HB3	59:BS:89:HIS:CD2	2.43	0.43
65:BY:25:ARG:HA	65:BY:26:PRO:HD2	1.74	0.43
68:Bc:101:ILE:HG12	68:Bc:127:PHE:CZ	2.53	0.43
71:Bf:128:GLN:O	71:Bf:132:ARG:HG2	2.17	0.43
72:Bg:26:LEU:HD21	72:Bg:29:LEU:CD1	2.48	0.43
75:Bj:160:LEU:O	75:Bj:252:HIS:HA	2.18	0.43
75:Bj:264:LEU:HA	75:Bj:264:LEU:HD12	1.81	0.43
88:Bz:601:UNK:O	88:Bz:604:UNK:HG3	2.19	0.43
1:AA:750:G:N2	1:AA:776:A:N7	2.67	0.43
1:AA:825:C:O2'	1:AA:826:C:O5'	2.33	0.43
1:AA:861:A:C2	1:AA:910:G:C6	3.07	0.43
3:AC:89:ASP:O	3:AC:93:ARG:HG2	2.19	0.43
4:AE:238:LYS:HB2	4:AE:238:LYS:HE3	1.67	0.43
13:AP:93:LEU:HD21	13:AP:103:MET:HE1	2.00	0.43
13:AP:95:GLY:O	28:Aj:167:PRO:HB2	2.19	0.43
19:Aa:264:THR:HG22	19:Aa:266:HIS:H	1.84	0.43
21:Ac:141:CYS:HB3	21:Ac:149:CYS:HB2	2.00	0.43
23:Ae:150:UNK:HG3	23:Ae:158:UNK:HB1	2.01	0.43
32:Ao:67:LYS:HB2	32:Ao:67:LYS:HE3	1.66	0.43
32:Ao:356:UNK:O	32:Ao:360:UNK:HG3	2.18	0.43
38:B2:66:LEU:HD12	38:B2:66:LEU:HA	1.87	0.43
38:B2:75:ASN:HD22	38:B2:75:ASN:HA	1.62	0.43
38:B2:158:LEU:HD12	38:B2:158:LEU:HA	1.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:B2:236:LEU:HD13	65:BY:48:PRO:HG3	2.01	0.43
39:B3:76:LYS:NZ	46:BA:472:G:C8	2.81	0.43
42:B6:44:LEU:HA	42:B6:54:VAL:O	2.19	0.43
45:B9:92:ASN:HB3	45:B9:94:LYS:HG2	2.01	0.43
46:BA:163:A:C2'	61:BU:35:LYS:HZ1	2.30	0.43
46:BA:209:A:H2'	46:BA:210:U:C6	2.54	0.43
46:BA:794:U:H4'	60:BT:260:TRP:HZ3	1.83	0.43
46:BA:956:U:H6	46:BA:956:U:H2'	1.57	0.43
46:BA:1048:C:H5'	46:BA:1049:G:OP1	2.19	0.43
52:BJ:140:TYR:HB3	52:BJ:143:LEU:HD12	2.01	0.43
56:BP:180:ASP:HB3	56:BP:204:MET:HB2	2.00	0.43
57:BQ:121:LEU:N	57:BQ:162:GLU:O	2.52	0.43
59:BS:145:VAL:HG22	59:BS:174:GLU:HB2	1.99	0.43
61:BU:29:ARG:HA	61:BU:29:ARG:HD3	1.72	0.43
65:BY:23:MET:HB3	65:BY:23:MET:HE2	1.89	0.43
65:BY:107:THR:HG22	65:BY:109:ILE:HG13	2.00	0.43
66:Ba:149:ASN:HB2	66:Ba:152:GLU:HB3	2.01	0.43
66:Ba:195:HIS:O	66:Ba:197:SER:N	2.44	0.43
72:Bg:34:SER:HB2	72:Bg:37:ALA:H	1.83	0.43
86:Bw:91:TYR:CE2	86:Bw:269:LYS:HE3	2.53	0.43
87:Bx:78:LYS:HG2	87:Bx:79:HIS:CD2	2.54	0.43
88:Bz:407:UNK:O	88:Bz:411:UNK:HG3	2.19	0.43
1:AA:318:C:C3'	15:AR:106:LYS:HZ3	2.29	0.43
1:AA:561:U:H1'	1:AA:711:A:H62	1.83	0.43
1:AA:871:U:H3	1:AA:896:A:H61	1.66	0.43
2:AB:262:LYS:O	2:AB:266:VAL:HG23	2.19	0.43
4:AE:401:VAL:HG22	21:Ac:15:TYR:CE1	2.54	0.43
6:AG:81:LYS:HB2	6:AG:81:LYS:HE3	1.75	0.43
6:AG:120:ARG:HG3	25:Ag:364:TRP:HH2	1.83	0.43
9:AK:88:ALA:HB3	9:AK:151:VAL:HG23	2.00	0.43
23:Ae:242:UNK:O	23:Ae:242:UNK:HG2	2.19	0.43
28:Aj:58:VAL:HG22	28:Aj:137:HIS:ND1	2.34	0.43
32:Ao:108:LEU:HD12	32:Ao:108:LEU:HA	1.88	0.43
33:Ap:113:LEU:HD12	33:Ap:113:LEU:HA	1.86	0.43
37:B1:143:PHE:O	37:B1:147:LYS:N	2.47	0.43
39:B3:66:LEU:HA	39:B3:66:LEU:HD23	1.74	0.43
42:B6:37:LEU:HD21	42:B6:40:LYS:HE3	2.01	0.43
46:BA:431:A:H4'	46:BA:432:G:OP2	2.18	0.43
46:BA:656:U:H2'	46:BA:657:U:O4'	2.18	0.43
46:BA:737:U:H2'	46:BA:738:U:C6	2.54	0.43
46:BA:904:G:C2	46:BA:914:C:C2	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:BA:1314:U:H2'	46:BA:1315:A:O4'	2.19	0.43
46:BA:1330:G:C2	46:BA:1401:U:O2	2.72	0.43
49:BE:219:MET:O	49:BE:223:GLY:N	2.51	0.43
52:BJ:41:HIS:CD2	52:BJ:43:GLU:H	2.36	0.43
53:BK:111:LEU:HD12	53:BK:154:ARG:HB3	2.01	0.43
56:BP:210:LEU:HD23	56:BP:210:LEU:HA	1.81	0.43
56:BP:280:LYS:HA	77:Bl:45:TYR:CZ	2.53	0.43
66:Ba:105:TYR:CZ	66:Ba:262:THR:HG21	2.53	0.43
66:Ba:373:LEU:HD12	66:Ba:373:LEU:HA	1.87	0.43
67:Bb:31:PRO:HB3	67:Bb:35:MET:HE2	2.00	0.43
73:Bh:101:GLU:OE1	73:Bh:104:LYS:NZ	2.44	0.43
73:Bh:216:ARG:HA	73:Bh:220:ILE:HG13	2.01	0.43
73:Bh:238:MET:O	73:Bh:241:LEU:HB3	2.19	0.43
86:Bw:265:LEU:HB3	86:Bw:266:PRO:C	2.43	0.43
86:Bw:362:SER:OG	86:Bw:392:SER:HA	2.19	0.43
1:AA:64:C:H2'	22:Ad:30:ARG:HA	2.00	0.43
1:AA:898:A:H3'	1:AA:898:A:N3	2.33	0.43
6:AG:168:TYR:HB3	6:AG:236:LEU:HD13	2.00	0.43
19:Aa:154:LYS:NZ	19:Aa:181:ARG:NH1	2.66	0.43
19:Aa:198:ARG:NH1	33:Ap:173:ARG:HB2	2.34	0.43
19:Aa:337:UNK:HG2	19:Aa:337:UNK:O	2.19	0.43
21:Ac:63:GLN:HE21	21:Ac:63:GLN:HB3	1.63	0.43
23:Ae:108:UNK:HG2	23:Ae:109:UNK:N	2.32	0.43
25:Ag:79:PRO:HG2	25:Ag:193:ALA:CA	2.49	0.43
25:Ag:127:GLY:O	25:Ag:322:TYR:HB2	2.17	0.43
26:Ah:296:TRP:HB3	26:Ah:302:LEU:HB2	2.01	0.43
28:Aj:61:GLU:HG3	28:Aj:62:SER:H	1.84	0.43
29:Ak:63:ALA:HB3	29:Ak:66:GLN:HB2	2.00	0.43
32:Ao:92:ASP:OD1	32:Ao:92:ASP:N	2.52	0.43
32:Ao:280:UNK:O	32:Ao:283:UNK:HG3	2.19	0.43
32:Ao:374:UNK:CA	32:Ao:377:UNK:HG3	2.48	0.43
32:Ao:424:UNK:HB2	32:Ao:462:UNK:CG	2.48	0.43
38:B2:95:LYS:NZ	65:BY:181:ASP:O	2.51	0.43
46:BA:37:A:C8	70:Be:37:LYS:HD3	2.54	0.43
46:BA:642:G:O6	63:BW:81:SER:HB2	2.18	0.43
49:BE:56:GLU:O	49:BE:59:PRO:HD2	2.18	0.43
55:BO:42:ASP:HB3	55:BO:119:ILE:HG12	2.01	0.43
55:BO:58:ILE:HD12	55:BO:74:LEU:HG	2.01	0.43
60:BT:82:PRO:HA	60:BT:83:PRO:HD3	1.88	0.43
64:BX:139:PRO:O	74:Bi:280:VAL:HG11	2.19	0.43
65:BY:188:VAL:HA	65:BY:189:PRO:HD3	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:BY:215:TRP:O	66:Ba:64:MET:HE1	2.18	0.43
66:Ba:146:HIS:HB3	66:Ba:150:GLN:HG3	2.01	0.43
66:Ba:408:PRO:HB2	66:Ba:412:ARG:NH2	2.34	0.43
67:Bb:136:ARG:NH1	67:Bb:139:TRP:CZ3	2.87	0.43
67:Bb:203:GLU:CD	84:Bu:194:SER:HB3	2.44	0.43
79:Bn:80:LEU:HD23	79:Bn:80:LEU:HA	1.81	0.43
86:Bw:395:LEU:HA	86:Bw:411:VAL:HG21	2.00	0.43
88:Bz:21:UNK:HA	88:Bz:24:UNK:CG	2.45	0.43
2:AB:66:LEU:HD23	2:AB:133:HIS:HE1	1.84	0.43
5:AF:65:LEU:HD21	15:AR:76:LYS:HD3	2.01	0.43
7:AI:321:LEU:HB3	7:AI:323:ARG:HD2	1.99	0.43
13:AP:111:ARG:CZ	19:Aa:146:ILE:HG22	2.48	0.43
16:AU:50:ARG:HH11	16:AU:50:ARG:HG2	1.83	0.43
16:AU:50:ARG:HD2	16:AU:50:ARG:HA	1.53	0.43
17:AV:43:Y5P:H2'	17:AV:44:Y5P:H6	2.01	0.43
17:AY:29:Y5P:H2'	17:AY:30:Y5P:O4'	2.19	0.43
19:Aa:96:GLU:H	19:Aa:96:GLU:HG3	1.66	0.43
23:Ae:223:UNK:O	23:Ae:226:UNK:HG3	2.19	0.43
23:Ae:246:UNK:CG	23:Ae:272:UNK:HG1	2.47	0.43
29:Ak:72:TYR:OH	29:Ak:78:PHE:HA	2.19	0.43
32:Ao:497:UNK:CA	32:Ao:500:UNK:HG3	2.48	0.43
32:Ao:514:UNK:O	32:Ao:518:UNK:HB1	2.19	0.43
35:Az:702:UNK:HA	35:Az:705:UNK:CG	2.48	0.43
37:B1:92:VAL:CG2	37:B1:98:SER:HB3	2.48	0.43
37:B1:202:GLU:OE1	37:B1:214:LYS:NZ	2.34	0.43
38:B2:80:LYS:HZ3	74:Bi:71:ARG:NH2	2.16	0.43
47:BB:28:P5P:O3'	69:Bd:133:ARG:NH2	2.37	0.43
49:BE:58:VAL:HB	49:BE:59:PRO:HD3	2.00	0.43
49:BE:203:TYR:CE1	49:BE:272:LYS:HB2	2.54	0.43
51:BI:118:VAL:O	51:BI:122:ARG:HB2	2.19	0.43
52:BJ:65:LEU:HD22	52:BJ:66:PRO:HD2	2.01	0.43
54:BN:67:PHE:HB2	54:BN:72:TRP:NE1	2.34	0.43
58:BR:131:LEU:HD23	58:BR:131:LEU:HA	1.83	0.43
59:BS:39:VAL:HB	59:BS:42:GLU:HB2	2.01	0.43
59:BS:56:LEU:O	59:BS:60:ALA:N	2.51	0.43
59:BS:56:LEU:CB	59:BS:62:ALA:HB2	2.48	0.43
62:BV:116:ASP:OD2	72:Bg:121:THR:HG23	2.19	0.43
66:Ba:150:GLN:O	66:Ba:154:VAL:HG23	2.19	0.43
74:Bi:196:GLN:HE21	74:Bi:196:GLN:HB2	1.70	0.43
86:Bw:392:SER:O	86:Bw:393:LYS:HG3	2.19	0.43
86:Bw:413:LEU:O	86:Bw:417:GLN:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:203:G:H2'	1:AA:204:U:C6	2.53	0.42
1:AA:875:A:N6	28:Aj:17:ARG:NH1	2.67	0.42
2:AB:83:LEU:HB2	2:AB:117:LEU:HD13	2.00	0.42
3:AC:96:MET:HA	3:AC:96:MET:HE2	2.01	0.42
4:AE:325:ARG:HH21	4:AE:430:THR:C	2.27	0.42
4:AE:374:ARG:HB3	4:AE:377:CYS:HB2	2.00	0.42
6:AG:68:PHE:HB3	7:AI:367:GLN:HE21	1.84	0.42
23:Ae:243:UNK:HG1	23:Ae:245:UNK:CG	2.49	0.42
25:Ag:205:GLU:CD	25:Ag:248:ARG:HH12	2.27	0.42
32:Ao:427:UNK:O	32:Ao:430:UNK:HG3	2.19	0.42
37:B1:146:LEU:HA	37:B1:162:LYS:HE3	2.01	0.42
40:B4:51:ARG:NH2	69:Bd:101:ARG:HD3	2.34	0.42
46:BA:366:A:O2'	46:BA:367:A:OP2	2.29	0.42
46:BA:1049:G:C2	46:BA:1050:A:C8	3.08	0.42
50:BF:217:LEU:HB2	50:BF:256:HIS:ND1	2.34	0.42
52:BJ:162:LYS:O	52:BJ:166:ARG:HB2	2.19	0.42
53:BK:124:LYS:NZ	53:BK:124:LYS:HB3	2.31	0.42
54:BN:173:PRO:HG2	54:BN:176:TYR:HB2	2.01	0.42
60:BT:145:LEU:HD12	60:BT:145:LEU:HA	1.85	0.42
60:BT:260:TRP:CD1	60:BT:260:TRP:H	2.36	0.42
61:BU:41:LEU:H	61:BU:41:LEU:HG	1.25	0.42
62:BV:73:PRO:O	62:BV:77:THR:OG1	2.29	0.42
62:BV:91:ILE:CG2	62:BV:206:PRO:HA	2.49	0.42
76:Bk:55:GLY:O	76:Bk:58:ARG:HB3	2.19	0.42
78:Bm:105:LEU:HD23	78:Bm:105:LEU:HA	1.93	0.42
88:Bz:22:UNK:CG	88:Bz:23:UNK:N	2.82	0.42
88:Bz:405:UNK:CA	88:Bz:408:UNK:HG3	2.49	0.42
1:AA:30:A:C6	1:AA:31:U:C4	3.07	0.42
1:AA:302:U:O5'	1:AA:302:U:H6	2.03	0.42
3:AC:138:TYR:CE1	27:Ai:70:LEU:HD13	2.54	0.42
4:AE:289:THR:HG21	4:AE:308:GLN:H	1.84	0.42
5:AF:42:LEU:HB2	5:AF:63:TYR:HB3	2.01	0.42
8:AJ:157:LEU:HD23	8:AJ:157:LEU:HA	1.83	0.42
13:AP:19:ILE:HG23	13:AP:51:LEU:HD12	2.00	0.42
13:AP:110:LEU:O	13:AP:113:LYS:HG2	2.20	0.42
13:AP:114:ARG:HD2	13:AP:114:ARG:HA	1.79	0.42
17:AV:43:Y5P:C4	17:AV:44:Y5P:H4	2.47	0.42
25:Ag:338:PRO:HD3	29:Ak:294:TYR:OH	2.19	0.42
29:Ak:136:PRO:HB3	32:Ao:58:VAL:O	2.19	0.42
37:B1:72:PRO:O	37:B1:75:SER:HB3	2.19	0.42
38:B2:197:ASN:HD22	38:B2:197:ASN:HA	1.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:B8:113:ARG:HD2	56:BP:75:TYR:O	2.19	0.42
46:BA:57:A:H5'	46:BA:57:A:H8	1.84	0.42
46:BA:194:G:H21	61:BU:44:ARG:NH2	2.17	0.42
46:BA:1154:A:H2'	46:BA:1155:C:O4'	2.19	0.42
51:BI:55:ILE:O	51:BI:83:VAL:HG22	2.20	0.42
58:BR:16:ARG:HH11	58:BR:47:ALA:HB1	1.84	0.42
59:BS:89:HIS:HA	59:BS:119:THR:CG2	2.49	0.42
61:BU:11:ARG:CZ	61:BU:13:ARG:HD2	2.49	0.42
61:BU:79:HIS:HE1	72:Bg:135:ASN:ND2	2.17	0.42
64:BX:10:TYR:CE1	70:Be:53:GLU:HB2	2.54	0.42
64:BX:64:PRO:HG2	64:BX:103:GLN:NE2	2.32	0.42
64:BX:149:GLY:HA2	74:Bi:273:LYS:NZ	2.34	0.42
67:Bb:87:ARG:HD3	67:Bb:87:ARG:HA	1.82	0.42
68:Bc:310:ASN:HD22	68:Bc:310:ASN:HA	1.71	0.42
71:Bf:106:GLY:O	71:Bf:110:GLU:HG3	2.19	0.42
75:Bj:46:ARG:HB3	75:Bj:229:ALA:CB	2.47	0.42
79:Bn:102:MET:HE2	79:Bn:102:MET:HB3	1.78	0.42
86:Bw:167:ALA:HB3	86:Bw:295:LEU:HD21	2.01	0.42
86:Bw:390:THR:HG22	86:Bw:391:GLN:O	2.19	0.42
87:Bx:129:PRO:O	87:Bx:132:ARG:HG3	2.20	0.42
1:AA:317:A:H2	1:AA:318:C:C5	2.37	0.42
1:AA:670:A:N7	92:AA:8087:HOH:O	2.37	0.42
1:AA:811:U:C5'	8:AJ:131:ARG:NH1	2.82	0.42
1:AA:961:C:OP1	30:Am:34:GLY:HA3	2.20	0.42
2:AB:221:ILE:HA	2:AB:235:VAL:HG13	2.01	0.42
4:AE:243:VAL:HG11	4:AE:268:PHE:CE1	2.54	0.42
10:AL:45:PRO:HA	10:AL:46:PRO:HD3	1.93	0.42
12:AO:86:VAL:HG22	22:Ad:161:GLN:NE2	2.35	0.42
15:AR:87:PRO:HA	15:AR:126:LYS:HB2	2.01	0.42
19:Aa:326:UNK:HA	19:Aa:329:UNK:HG3	2.00	0.42
22:Ad:48:VAL:HG11	33:Ap:220:TYR:CE2	2.55	0.42
23:Ae:39:UNK:O	23:Ae:39:UNK:HG2	2.17	0.42
23:Ae:267:UNK:O	23:Ae:270:UNK:CG	2.68	0.42
23:Ae:278:UNK:C	23:Ae:281:UNK:HG3	2.49	0.42
25:Ag:372:THR:HG22	25:Ag:373:GLU:H	1.85	0.42
32:Ao:532:UNK:HG2	32:Ao:533:UNK:N	2.33	0.42
33:Ap:103:ASN:HA	33:Ap:104:PRO:HD3	1.87	0.42
38:B2:134:LEU:HD12	38:B2:134:LEU:HA	1.72	0.42
39:B3:81:TRP:CD1	39:B3:82:GLU:HG2	2.54	0.42
46:BA:27:A:H2'	46:BA:28:A:C8	2.53	0.42
46:BA:924:U:HO2'	46:BA:925:A:P	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:BA:1494:C:OP1	49:BE:213:LYS:HE2	2.19	0.42
48:BD:75:MET:HE2	48:BD:75:MET:HB3	1.93	0.42
48:BD:86:ASN:ND2	48:BD:90:GLN:HB2	2.28	0.42
50:BF:66:ILE:HD13	50:BF:263:LEU:HD11	2.00	0.42
54:BN:24:LYS:HB3	54:BN:24:LYS:HE2	1.76	0.42
56:BP:118:LEU:HB3	56:BP:187:LEU:HD21	2.02	0.42
56:BP:156:VAL:O	56:BP:176:THR:HA	2.19	0.42
56:BP:184:LEU:O	56:BP:187:LEU:HB3	2.18	0.42
59:BS:48:PHE:CZ	67:Bb:223:GLY:HA2	2.54	0.42
60:BT:209:GLN:HE21	60:BT:211:PHE:HA	1.84	0.42
63:BW:49:TRP:CD1	63:BW:74:CYS:HG	2.37	0.42
67:Bb:35:MET:HG3	67:Bb:36:PRO:HD2	2.00	0.42
67:Bb:258:PHE:N	67:Bb:258:PHE:CD1	2.86	0.42
68:Bc:193:LYS:HA	68:Bc:196:LEU:HD12	1.99	0.42
71:Bf:68:PRO:HG2	71:Bf:71:HIS:CG	2.53	0.42
71:Bf:113:SER:HB2	71:Bf:118:THR:O	2.19	0.42
72:Bg:11:LEU:HD22	72:Bg:118:PRO:O	2.18	0.42
73:Bh:215:ILE:HD13	73:Bh:215:ILE:HA	1.85	0.42
73:Bh:245:LEU:HD22	73:Bh:250:ILE:HB	2.01	0.42
80:Bo:31:GLN:HB3	80:Bo:33:PHE:CE1	2.55	0.42
86:Bw:77:ASP:O	86:Bw:81:ARG:HB2	2.20	0.42
86:Bw:278:ILE:HD12	86:Bw:336:TYR:CD2	2.54	0.42
1:AA:527:G:N2	1:AA:839:C:C2	2.88	0.42
1:AA:581:A:N7	1:AA:802:A:H2	2.17	0.42
1:AA:685:C:C3'	1:AA:686:A:H5'	2.48	0.42
1:AA:959:U:O4	30:Am:24:ASN:HB3	2.18	0.42
4:AE:130:GLN:HE21	4:AE:176:ARG:HH22	1.68	0.42
4:AE:320:ILE:HG12	4:AE:349:LEU:HD22	2.01	0.42
8:AJ:122:LYS:HG3	8:AJ:132:VAL:HG22	2.02	0.42
13:AP:102:MET:HE1	22:Ad:56:LEU:HD13	2.01	0.42
19:Aa:327:UNK:HG2	19:Aa:328:UNK:N	2.35	0.42
23:Ae:28:UNK:CB	23:Ae:369:UNK:HG3	2.50	0.42
23:Ae:216:UNK:HA	23:Ae:219:UNK:HG3	2.02	0.42
23:Ae:249:UNK:HG2	23:Ae:250:UNK:N	2.35	0.42
25:Ag:83:PRO:HA	25:Ag:84:PRO:HD3	1.81	0.42
25:Ag:93:PHE:C	25:Ag:95:GLU:H	2.27	0.42
28:Aj:188:GLU:CD	33:Ap:191:PRO:HG3	2.45	0.42
29:Ak:223:TYR:HA	29:Ak:226:TYR:HB3	2.00	0.42
30:Am:52:MET:HB3	30:Am:52:MET:HE2	1.75	0.42
36:B0:43:GLY:C	36:B0:45:LYS:H	2.26	0.42
37:B1:96:LYS:O	37:B1:96:LYS:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:B1:163:ARG:CZ	66:Ba:55:LEU:HD11	2.49	0.42
38:B2:122:LYS:NZ	38:B2:122:LYS:HB3	2.35	0.42
45:B9:81:ARG:NH1	46:BA:1523:C:C5	2.88	0.42
45:B9:84:ARG:NH1	45:B9:99:GLN:O	2.53	0.42
46:BA:83:A:H4'	46:BA:84:G:O5'	2.18	0.42
46:BA:129:A:H2'	46:BA:130:A:C8	2.54	0.42
46:BA:482:U:P	80:Bo:25:SER:HB3	2.58	0.42
46:BA:1519:U:H3'	46:BA:1520:A:H5'	2.01	0.42
50:BF:67:GLU:HA	50:BF:75:GLU:O	2.19	0.42
50:BF:67:GLU:O	50:BF:190:VAL:HA	2.19	0.42
50:BF:243:VAL:HG22	50:BF:244:PRO:O	2.19	0.42
54:BN:7:ALA:N	54:BN:8:PRO:HD2	2.34	0.42
58:BR:83:LYS:HG3	86:Bw:45:PRO:HG2	2.00	0.42
58:BR:109:GLN:NE2	58:BR:120:LYS:HG3	2.35	0.42
59:BS:115:HIS:HD2	67:Bb:135:VAL:HG22	1.85	0.42
61:BU:67:LEU:HD21	61:BU:71:ARG:NH1	2.34	0.42
64:BX:16:GLN:OE1	70:Be:53:GLU:HA	2.19	0.42
67:Bb:379:ILE:HG13	67:Bb:380:TYR:CD1	2.54	0.42
68:Bc:163:LEU:H	68:Bc:230:ASN:HD21	1.66	0.42
69:Bd:94:PHE:N	69:Bd:94:PHE:CD1	2.87	0.42
73:Bh:93:VAL:HG22	73:Bh:180:LEU:HD12	2.01	0.42
76:Bk:100:MET:HG2	76:Bk:153:HIS:CD2	2.55	0.42
78:Bm:141:PHE:O	78:Bm:145:ILE:HG13	2.20	0.42
83:Bt:25:ARG:HA	83:Bt:26:PRO:HD3	1.78	0.42
83:Bt:49:LEU:HD12	83:Bt:49:LEU:HA	1.74	0.42
85:Bv:107:GLN:HG3	85:Bv:108:LEU:N	2.34	0.42
87:Bx:157:ARG:HE	87:Bx:157:ARG:HB3	1.48	0.42
1:AA:432:A:O2'	1:AA:434:A:N7	2.47	0.42
1:AA:658:C:H2'	1:AA:659:A:O4'	2.19	0.42
1:AA:708:A:H5'	1:AA:709:A:OP1	2.19	0.42
4:AE:255:GLY:HA3	4:AE:278:TYR:O	2.19	0.42
6:AG:59:THR:HG22	6:AG:63:LYS:HE3	2.00	0.42
11:AN:102:ARG:HH11	11:AN:102:ARG:HG3	1.84	0.42
13:AP:65:LEU:HD12	21:Ac:146:GLN:HE22	1.84	0.42
14:AQ:32:ARG:HG2	21:Ac:63:GLN:HG3	2.00	0.42
17:AY:54:Y5P:HB2	57:BQ:106:ARG:NH2	2.34	0.42
26:Ah:292:GLU:HG3	26:Ah:296:TRP:NE1	2.35	0.42
29:Ak:272:LYS:HA	29:Ak:272:LYS:HD3	1.78	0.42
42:B6:38:ARG:HG3	42:B6:39:GLU:N	2.34	0.42
46:BA:63:A:C6	79:Bn:118:TYR:CD2	3.08	0.42
46:BA:521:U:O2	46:BA:530:A:H5'	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:BA:570:A:C6	46:BA:571:A:C6	3.08	0.42
54:BN:46:VAL:HB	63:BW:206:ILE:HG23	2.02	0.42
57:BQ:96:TYR:HE1	57:BQ:153:PRO:HG3	1.84	0.42
59:BS:137:LEU:HD11	59:BS:168:GLY:O	2.19	0.42
61:BU:16:ASP:OD1	61:BU:16:ASP:N	2.30	0.42
66:Ba:79:ASP:HA	66:Ba:80:PRO:HD2	1.87	0.42
66:Ba:256:PHE:HB2	66:Ba:259:ILE:HD12	2.02	0.42
66:Ba:340:VAL:O	66:Ba:358:GLN:HA	2.20	0.42
67:Bb:47:ARG:HG3	76:Bk:120:LYS:NZ	2.32	0.42
67:Bb:257:PRO:HB3	67:Bb:268:PHE:CZ	2.54	0.42
73:Bh:227:GLU:HB2	73:Bh:230:GLU:HB2	2.02	0.42
74:Bi:240:ARG:CZ	74:Bi:274:GLN:HG3	2.49	0.42
75:Bj:140:ALA:HA	75:Bj:143:LYS:HA	2.01	0.42
86:Bw:103:ASP:N	86:Bw:103:ASP:OD1	2.52	0.42
88:Bz:99:UNK:H2	88:Bz:300:UNK:HG3	1.85	0.42
1:AA:102:G:H5'	14:AQ:75:LYS:NZ	2.35	0.42
1:AA:937:A:H2'	1:AA:938:U:C6	2.54	0.42
2:AB:117:LEU:HA	2:AB:120:THR:HB	2.01	0.42
4:AE:193:TRP:CE3	4:AE:199:GLY:HA3	2.55	0.42
12:AO:127:GLU:CD	12:AO:178:VAL:HG11	2.44	0.42
14:AQ:18:ILE:HD13	14:AQ:18:ILE:HA	1.93	0.42
14:AQ:98:LYS:HD2	14:AQ:107:GLU:O	2.20	0.42
17:AY:74:Y5P:HB2	17:AY:74:Y5P:H6	2.00	0.42
20:Ab:125:LEU:HD23	20:Ab:125:LEU:HA	1.89	0.42
23:Ae:131:UNK:HB2	23:Ae:136:UNK:HB2	2.01	0.42
24:Af:157:ALA:HB2	30:Am:113:ASN:HD21	1.84	0.42
25:Ag:158:HIS:CD2	25:Ag:266:ALA:HB2	2.55	0.42
25:Ag:382:LEU:HB3	25:Ag:393:LEU:HD13	2.01	0.42
26:Ah:302:LEU:HD22	26:Ah:303:TRP:H	1.84	0.42
27:Ai:74:GLU:CD	27:Ai:74:GLU:H	2.26	0.42
32:Ao:228:UNK:O	32:Ao:232:UNK:HB1	2.20	0.42
32:Ao:513:UNK:O	32:Ao:517:UNK:HB1	2.19	0.42
36:B0:140:GLY:HA3	67:Bb:344:PHE:CZ	2.54	0.42
39:B3:65:LYS:HG3	83:Bt:53:PHE:CZ	2.54	0.42
42:B6:19:LYS:HG3	42:B6:30:PHE:CE2	2.54	0.42
44:B8:119:SER:OG	44:B8:183:ARG:HD3	2.20	0.42
46:BA:58:C:O5'	46:BA:58:C:H6	2.03	0.42
46:BA:207:A:H2'	46:BA:208:A:O4'	2.20	0.42
46:BA:538:A:H2	53:BK:38:ILE:HG12	1.83	0.42
46:BA:686:A:C3'	46:BA:687:A:H4'	2.49	0.42
46:BA:998:A:H2'	46:BA:999:A:C8	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:BA:1280:A:C6	46:BA:1315:A:C2	3.08	0.42
46:BA:1436:U:H2'	46:BA:1437:C:H6	1.84	0.42
46:BA:1455:A:O4'	46:BA:1457:U:H1'	2.20	0.42
46:BA:1482:C:C2	46:BA:1494:C:N4	2.87	0.42
46:BA:1556:U:H4'	58:BR:11:HIS:CG	2.55	0.42
47:BB:9:P5P:H5'2	47:BB:47:P5P:H1'	2.01	0.42
48:BD:83:GLY:O	48:BD:85:ARG:HG2	2.18	0.42
52:BJ:53:TYR:HB2	57:BQ:251:VAL:CG2	2.50	0.42
53:BK:33:PRO:HA	53:BK:37:PRO:HD2	2.02	0.42
54:BN:40:GLN:OE1	54:BN:113:PRO:HD3	2.19	0.42
54:BN:119:ARG:HD3	54:BN:119:ARG:HA	1.86	0.42
56:BP:83:PHE:C	56:BP:85:GLU:H	2.28	0.42
62:BV:170:SER:HB2	62:BV:194:GLN:CD	2.44	0.42
64:BX:63:VAL:HA	64:BX:64:PRO:HD3	1.70	0.42
69:Bd:173:ARG:HB3	76:Bk:184:LEU:HD23	2.02	0.42
70:Be:32:LYS:HB3	70:Be:32:LYS:HE2	1.76	0.42
71:Bf:48:GLU:O	71:Bf:60:CYS:HA	2.19	0.42
71:Bf:68:PRO:HG2	71:Bf:71:HIS:CD2	2.54	0.42
78:Bm:91:SER:HB2	78:Bm:123:ARG:NH1	2.35	0.42
82:Bq:103:PRO:HG2	82:Bq:105:LYS:CE	2.50	0.42
86:Bw:105:TRP:O	86:Bw:108:SER:HB3	2.20	0.42
87:Bx:116:GLU:HG2	87:Bx:120:LYS:HE3	2.01	0.42
88:Bz:406:UNK:O	88:Bz:409:UNK:HG3	2.20	0.42
88:Bz:604:UNK:HG2	88:Bz:605:UNK:N	2.34	0.42
1:AA:419:A:N6	1:AA:420:A:N1	2.68	0.42
4:AE:323:ILE:O	4:AE:327:ILE:HG13	2.20	0.42
7:AI:224:ARG:HG3	16:AU:85:GLN:HE22	1.83	0.42
13:AP:41:CYS:HB2	13:AP:42:PRO:HD2	2.02	0.42
17:AV:36:P5P:N1	18:AX:16:Y5P:N3	2.67	0.42
22:Ad:144:ARG:HA	22:Ad:147:GLN:CD	2.44	0.42
23:Ae:75:UNK:O	23:Ae:75:UNK:HG2	2.19	0.42
23:Ae:125:UNK:HG2	23:Ae:126:UNK:N	2.33	0.42
23:Ae:221:UNK:HB1	23:Ae:252:UNK:HB1	2.01	0.42
23:Ae:223:UNK:HA	23:Ae:226:UNK:HG3	2.02	0.42
23:Ae:274:UNK:HG2	23:Ae:275:UNK:N	2.34	0.42
23:Ae:406:UNK:O	23:Ae:407:UNK:HG3	2.19	0.42
31:An:193:LYS:HG3	31:An:193:LYS:O	2.20	0.42
32:Ao:481:UNK:O	32:Ao:484:UNK:HG3	2.19	0.42
33:Ap:120:VAL:O	33:Ap:124:GLU:HB2	2.20	0.42
37:B1:81:GLY:O	37:B1:130:ARG:NH1	2.52	0.42
42:B6:42:THR:CG2	42:B6:55:LEU:HD13	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:B7:50:LYS:HE2	43:B7:50:LYS:HB3	1.89	0.42
44:B8:169:ARG:HD2	44:B8:170:ASN:H	1.84	0.42
45:B9:78:LEU:HD13	45:B9:87:ILE:CD1	2.48	0.42
46:BA:215:C:O2	46:BA:219:G:H5"	2.19	0.42
46:BA:723:C:N4	66:Ba:389:LEU:HB2	2.34	0.42
46:BA:826:G:C2	46:BA:839:A:C2	3.07	0.42
46:BA:1506:A:H2	46:BA:1536:A:N7	2.16	0.42
49:BE:221:ARG:NH1	49:BE:259:GLY:CA	2.82	0.42
50:BF:108:ARG:HG2	50:BF:161:TYR:CD1	2.54	0.42
50:BF:126:LYS:HG3	50:BF:127:PRO:HD2	2.01	0.42
56:BP:230:PRO:HB3	84:Bu:60:ARG:O	2.20	0.42
61:BU:94:GLN:HE22	61:BU:146:VAL:N	2.18	0.42
61:BU:129:ALA:HB2	62:BV:68:ILE:HD12	2.01	0.42
64:BX:3:ARG:O	64:BX:4:ASN:HB2	2.19	0.42
69:Bd:129:HIS:O	69:Bd:133:ARG:HG3	2.20	0.42
69:Bd:173:ARG:HG2	76:Bk:175:HIS:HB2	2.00	0.42
72:Bg:103:LYS:HD3	72:Bg:103:LYS:HA	1.75	0.42
78:Bm:61:TYR:HB3	78:Bm:135:VAL:HG12	2.02	0.42
82:Bq:103:PRO:HA	82:Bq:104:PRO:HD3	1.89	0.42
86:Bw:94:TYR:HA	86:Bw:95:PRO:HD3	1.83	0.42
88:Bz:24:UNK:O	88:Bz:27:UNK:CG	2.45	0.42
88:Bz:302:UNK:CG	88:Bz:303:UNK:N	2.83	0.42
1:AA:87:U:H2'	1:AA:88:C:C6	2.54	0.42
2:AB:100:PHE:CZ	20:Ab:47:ARG:HD2	2.55	0.42
4:AE:287:ASP:O	4:AE:330:LYS:HE3	2.20	0.42
8:AJ:166:GLU:OE1	8:AJ:166:GLU:N	2.40	0.42
19:Aa:207:VAL:HG12	19:Aa:213:ASN:HD21	1.84	0.42
21:Ac:129:PHE:CE2	21:Ac:137:ARG:HG3	2.55	0.42
23:Ae:239:UNK:HG2	23:Ae:241:UNK:HG3	2.01	0.42
23:Ae:278:UNK:HA	23:Ae:281:UNK:CG	2.48	0.42
24:Af:153:ARG:NH1	24:Af:160:ASP:OD1	2.52	0.42
25:Ag:130:GLY:O	25:Ag:386:ASN:ND2	2.51	0.42
44:B8:98:SER:HB2	46:BA:76:G:O6	2.20	0.42
46:BA:96:U:C1'	46:BA:97:A:H5"	2.50	0.42
46:BA:149:A:H2'	46:BA:150:A:C8	2.55	0.42
46:BA:324:G:C6	46:BA:325:U:N3	2.87	0.42
46:BA:330:A:H8	46:BA:330:A:H5"	1.85	0.42
46:BA:353:U:H2'	46:BA:354:G:C8	2.54	0.42
46:BA:532:A:O2'	82:Bq:133:SER:O	2.37	0.42
46:BA:570:A:H4'	46:BA:570:A:OP1	2.19	0.42
46:BA:809:A:H1'	49:BE:230:THR:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:BA:1069:U:H5	46:BA:1417:C:C2	2.37	0.42
46:BA:1236:A:H5'	46:BA:1237:A:OP2	2.20	0.42
49:BE:122:LEU:HD13	49:BE:299:ILE:HD11	2.01	0.42
50:BF:199:ASP:HA	50:BF:200:PRO:HD2	1.94	0.42
51:BI:94:LEU:HB2	51:BI:116:LYS:HG2	2.01	0.42
53:BK:104:THR:HG21	53:BK:150:SER:HA	2.02	0.42
56:BP:11:ARG:NH1	56:BP:11:ARG:CG	2.76	0.42
57:BQ:214:THR:O	57:BQ:218:ILE:HG13	2.20	0.42
69:Bd:157:LEU:HD13	75:Bj:232:PHE:CE2	2.46	0.42
73:Bh:88:LEU:HD23	73:Bh:88:LEU:HA	1.92	0.42
74:Bi:84:ILE:HG23	74:Bi:247:VAL:HG11	2.02	0.42
74:Bi:150:LEU:HD23	74:Bi:153:ASN:HD22	1.85	0.42
76:Bk:168:GLU:O	76:Bk:172:GLU:HG3	2.19	0.42
83:Bt:96:LEU:HD22	83:Bt:99:ARG:HD2	2.01	0.42
84:Bu:134:LEU:HD11	84:Bu:156:MET:HE2	2.01	0.42
84:Bu:177:SER:O	84:Bu:181:ASN:HB2	2.20	0.42
86:Bw:335:MET:HE2	86:Bw:335:MET:HB3	1.85	0.42
1:AA:636:U:P	2:AB:213:LYS:NZ	2.92	0.42
4:AE:254:ALA:O	4:AE:280:HIS:N	2.33	0.42
7:AI:127:HIS:CD2	7:AI:128:PRO:HD2	2.55	0.42
12:AO:210:LEU:HD22	31:An:173:LEU:HD22	2.02	0.42
19:Aa:217:MET:SD	19:Aa:226:VAL:HG22	2.60	0.42
23:Ae:196:UNK:HG3	23:Ae:199:UNK:HB2	2.01	0.42
23:Ae:211:UNK:HB1	23:Ae:216:UNK:HG2	2.02	0.42
23:Ae:354:UNK:HG1	23:Ae:357:UNK:CG	2.45	0.42
29:Ak:68:TRP:N	29:Ak:69:PRO:HD2	2.35	0.42
29:Ak:268:LEU:O	29:Ak:272:LYS:HG2	2.19	0.42
33:Ap:60:ASP:CG	33:Ap:121:LYS:NZ	2.76	0.42
36:B0:76:HIS:HB2	36:B0:130:PHE:CD1	2.55	0.42
43:B7:74:ARG:HD3	43:B7:74:ARG:HA	1.71	0.42
46:BA:68:A:N3	46:BA:69:C:H5'	2.35	0.42
46:BA:210:U:H2'	46:BA:211:C:C6	2.54	0.42
46:BA:265:C:H5"	46:BA:266:A:H5'	2.00	0.42
46:BA:991:U:H2'	46:BA:992:A:C8	2.54	0.42
46:BA:1555:C:H4'	60:BT:86:ARG:HH12	1.85	0.42
49:BE:43:GLY:H	68:Bc:98:ARG:NH1	2.17	0.42
49:BE:80:LEU:O	49:BE:84:PRO:HG3	2.19	0.42
50:BF:108:ARG:HG2	50:BF:161:TYR:CE1	2.55	0.42
52:BJ:143:LEU:HD11	52:BJ:180:CYS:HB2	2.01	0.42
52:BJ:175:PRO:HG2	81:Bp:34:LEU:HD21	2.01	0.42
53:BK:87:VAL:HG12	53:BK:91:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:BN:28:PRO:HB3	54:BN:65:ILE:HD13	2.01	0.42
54:BN:174:GLU:HA	87:Bx:56:THR:CG2	2.47	0.42
58:BR:134:LEU:HD12	58:BR:134:LEU:HA	1.83	0.42
61:BU:39:TYR:O	61:BU:43:VAL:HG23	2.20	0.42
63:BW:101:LEU:HD23	63:BW:101:LEU:HA	1.82	0.42
66:Ba:78:TRP:CH2	66:Ba:80:PRO:HB3	2.55	0.42
67:Bb:366:LEU:HD23	67:Bb:366:LEU:HA	1.93	0.42
68:Bc:244:ASN:HA	68:Bc:245:PRO:HD3	1.85	0.42
73:Bh:188:PRO:N	73:Bh:189:PRO:HD2	2.35	0.42
76:Bk:133:GLU:O	88:Bz:104:UNK:N	2.53	0.42
78:Bm:69:SER:HA	78:Bm:72:GLU:HG2	2.01	0.42
79:Bn:94:LYS:O	79:Bn:98:VAL:HG23	2.20	0.42
81:Bp:68:PHE:CE1	81:Bp:94:ILE:HG13	2.54	0.42
1:AA:190:G:H21	1:AA:192:C:H41	1.67	0.42
1:AA:254:C:H4’	1:AA:261:A:C6	2.55	0.42
1:AA:450:C:O2’	1:AA:502:A:O2’	2.36	0.42
1:AA:454:A:H2’	1:AA:456:A:OP1	2.20	0.42
1:AA:460:A:H4’	1:AA:461:A:OP2	2.20	0.42
1:AA:650:A:N6	2:AB:176:THR:OG1	2.53	0.42
1:AA:881:A:C2	23:Ae:66:UNK:HG1	2.54	0.42
5:AF:22:LEU:O	5:AF:26:LEU:HG	2.19	0.42
7:AI:176:HIS:ND1	7:AI:233:PRO:HG2	2.34	0.42
17:AV:66:Y5P:H4A	17:AV:67:Y5P:N3	2.35	0.42
21:Ac:125:HIS:HA	21:Ac:126:PRO:HD3	1.76	0.42
25:Ag:66:UNK:O	25:Ag:66:UNK:CG	2.66	0.42
29:Ak:255:TRP:CD1	29:Ak:295:ARG:HG2	2.55	0.42
32:Ao:316:UNK:O	32:Ao:319:UNK:HG3	2.20	0.42
32:Ao:536:UNK:CB	32:Ao:579:UNK:HG1	2.50	0.42
32:Ao:601:UNK:CG	32:Ao:655:UNK:HB1	2.50	0.42
36:B0:64:GLY:N	36:B0:91:ALA:O	2.44	0.42
46:BA:328:A:OP1	48:BD:274:GLY:N	2.53	0.42
46:BA:365:A:N3	46:BA:365:A:H2’	2.35	0.42
46:BA:528:A:O2’	46:BA:545:A:N6	2.53	0.42
46:BA:1060:A:C2	46:BA:1062:G:C8	3.08	0.42
46:BA:1129:U:H2’	46:BA:1130:G:H8	1.85	0.42
47:BB:25:P5P:H8	47:BB:25:P5P:H5’1	2.01	0.42
49:BE:48:TRP:CD1	49:BE:50:ASP:H	2.38	0.42
49:BE:293:LYS:HB3	49:BE:293:LYS:HE2	1.78	0.42
52:BJ:53:TYR:HB2	57:BQ:251:VAL:HG22	2.02	0.42
54:BN:178:LEU:HD12	87:Bx:35:PHE:CE1	2.55	0.42
56:BP:169:LYS:HD3	84:Bu:143:PHE:HZ	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:BP:184:LEU:HD12	56:BP:184:LEU:HA	1.80	0.42
58:BR:38:ARG:HG2	58:BR:39:HIS:CD2	2.55	0.42
59:BS:117:TYR:HE1	67:Bb:114:ARG:HE	1.68	0.42
64:BX:98:GLN:OE1	86:Bw:100:LEU:HG	2.19	0.42
65:BY:62:VAL:HB	65:BY:120:VAL:HG13	2.02	0.42
65:BY:194:LEU:HD23	65:BY:195:GLU:OE2	2.20	0.42
68:Bc:157:ASP:OD1	68:Bc:157:ASP:N	2.51	0.42
73:Bh:118:ASN:HD22	73:Bh:118:ASN:HA	1.75	0.42
75:Bj:142:LYS:C	75:Bj:144:ASP:H	2.28	0.42
83:Bt:39:LEU:HD23	83:Bt:39:LEU:HA	1.74	0.42
83:Bt:87:ARG:HB2	83:Bt:90:GLU:OE1	2.20	0.42
87:Bx:70:CYS:O	87:Bx:73:CYS:N	2.47	0.42
87:Bx:86:VAL:O	87:Bx:89:LEU:N	2.53	0.42
87:Bx:155:SER:OG	87:Bx:157:ARG:HG2	2.20	0.42
88:Bz:409:UNK:O	88:Bz:412:UNK:CG	2.51	0.42
88:Bz:412:UNK:C	88:Bz:415:UNK:HG3	2.50	0.42
1:AA:4:C:C4	4:AE:427:ARG:HD3	2.55	0.41
1:AA:273:A:OP2	33:Ap:96:ARG:NH2	2.22	0.41
1:AA:305:A:H2'	1:AA:306:G:O4'	2.19	0.41
1:AA:462:A:C6	1:AA:463:U:C4	3.08	0.41
6:AG:131:ALA:HA	6:AG:134:GLN:HB2	2.02	0.41
7:AI:127:HIS:CD2	7:AI:129:GLU:HG2	2.54	0.41
8:AJ:68:GLU:HB2	32:Ao:62:LYS:HE2	2.02	0.41
10:AL:115:THR:HG22	10:AL:117:ASP:H	1.84	0.41
15:AR:79:GLN:HG3	15:AR:133:ASP:OD2	2.18	0.41
17:AY:8:Y5P:N3	17:AY:14:Y5P:H4	2.35	0.41
22:Ad:54:PHE:CD2	33:Ap:208:PRO:HB3	2.55	0.41
23:Ae:75:UNK:O	23:Ae:79:UNK:HG3	2.20	0.41
23:Ae:224:UNK:HA	23:Ae:227:UNK:CG	2.50	0.41
25:Ag:100:VAL:HG13	25:Ag:139:HIS:NE2	2.35	0.41
25:Ag:259:VAL:HG21	25:Ag:295:MET:SD	2.59	0.41
28:Aj:79:LEU:HB3	28:Aj:94:TYR:HB2	2.02	0.41
32:Ao:345:UNK:HA	32:Ao:348:UNK:HG3	2.01	0.41
41:B5:138:ARG:HA	41:B5:141:MET:HG2	2.01	0.41
43:B7:73:LEU:HD12	46:BA:31:A:H1'	2.02	0.41
44:B8:106:THR:OG1	44:B8:162:THR:HA	2.20	0.41
46:BA:389:A:H2'	46:BA:390:A:C8	2.56	0.41
53:BK:149:ARG:HH12	82:Bq:104:PRO:CD	2.32	0.41
54:BN:4:PHE:HE2	73:Bh:285:PRO:HD3	1.84	0.41
54:BN:74:GLN:HA	87:Bx:161:PRO:HA	2.02	0.41
55:BO:45:ALA:O	55:BO:49:THR:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:BP:204:MET:HA	56:BP:204:MET:HE2	2.02	0.41
63:BW:80:TYR:HD2	63:BW:85:MET:HE2	1.84	0.41
65:BY:81:ARG:HG2	65:BY:81:ARG:NH1	2.35	0.41
65:BY:177:THR:OG1	70:Be:69:LYS:HB2	2.19	0.41
67:Bb:286:ARG:NH1	67:Bb:295:GLN:O	2.52	0.41
73:Bh:231:MET:H	73:Bh:231:MET:HG2	1.52	0.41
73:Bh:259:ARG:NH1	73:Bh:259:ARG:CG	2.66	0.41
77:Bl:77:ASP:HB2	77:Bl:78:PRO:HD3	2.01	0.41
78:Bm:136:GLN:HB3	78:Bm:138:ARG:HG2	2.02	0.41
3:AC:58:ALA:HB3	3:AC:60:HIS:CE1	2.55	0.41
4:AE:93:LEU:H	27:Ai:75:HIS:CD2	2.38	0.41
4:AE:244:LEU:HD12	4:AE:257:ALA:O	2.20	0.41
6:AG:163:LYS:HE3	18:AX:12:Y5P:HA1	2.02	0.41
7:AI:116:LEU:O	7:AI:122:ARG:NH1	2.53	0.41
19:Aa:149:GLY:HA2	33:Ap:235:MET:HG3	2.01	0.41
21:Ac:152:LEU:H	21:Ac:152:LEU:HG	1.71	0.41
28:Aj:27:ARG:HA	28:Aj:28:PRO:HD3	1.89	0.41
29:Ak:164:SER:HB3	32:Ao:134:GLU:HG2	2.01	0.41
30:Am:113:ASN:O	30:Am:115:PRO:HD3	2.20	0.41
32:Ao:175:UNK:HA	32:Ao:178:UNK:CG	2.50	0.41
32:Ao:206:UNK:O	32:Ao:210:UNK:HG3	2.20	0.41
32:Ao:413:UNK:CA	32:Ao:416:UNK:HG3	2.45	0.41
32:Ao:424:UNK:HB2	32:Ao:462:UNK:HG1	2.01	0.41
37:B1:128:THR:HG22	37:B1:129:MET:H	1.85	0.41
41:B5:177:ARG:CG	41:B5:177:ARG:HH11	2.32	0.41
44:B8:94:VAL:HB	44:B8:96:TYR:CE1	2.56	0.41
46:BA:6:A:O2'	79:Bn:36:VAL:HG22	2.19	0.41
46:BA:642:G:O2'	46:BA:1005:G:O6	2.25	0.41
46:BA:715:A:H2'	46:BA:716:A:C8	2.55	0.41
46:BA:1149:G:C2	46:BA:1150:G:C4	3.08	0.41
46:BA:1355:C:H3'	46:BA:1356:G:H5"	2.02	0.41
47:BB:29:P5P:H2'	47:BB:30:P5P:C8	2.43	0.41
49:BE:297:VAL:HG12	49:BE:298:LYS:N	2.33	0.41
53:BK:103:HIS:HB3	53:BK:106:LYS:HD2	2.02	0.41
56:BP:176:THR:OG1	56:BP:219:ASN:O	2.38	0.41
57:BQ:97:LEU:HD11	57:BQ:160:ILE:HD12	2.02	0.41
57:BQ:194:THR:O	57:BQ:197:LYS:HB3	2.20	0.41
64:BX:16:GLN:NE2	64:BX:17:LEU:O	2.49	0.41
64:BX:144:VAL:HG11	74:Bi:233:TYR:CD1	2.56	0.41
67:Bb:27:ARG:HD2	67:Bb:27:ARG:HA	1.83	0.41
71:Bf:51:LEU:HD12	71:Bf:57:THR:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:Bo:110:LEU:HD12	80:Bo:110:LEU:HA	1.91	0.41
87:Bx:89:LEU:HD23	87:Bx:89:LEU:HA	1.78	0.41
88:Bz:24:UNK:CA	88:Bz:27:UNK:HG3	2.50	0.41
2:AB:84:PHE:HD1	24:Af:81:PHE:HE1	1.67	0.41
3:AC:148:LYS:NZ	32:Ao:141:MET:HE3	2.35	0.41
6:AG:155:VAL:H	6:AG:227:HIS:HE1	1.67	0.41
8:AJ:135:GLU:HB2	11:AN:126:ALA:HB2	2.03	0.41
10:AL:64:ARG:HG3	10:AL:66:PHE:CD2	2.54	0.41
12:AO:133:LEU:HD23	12:AO:133:LEU:HA	1.83	0.41
13:AP:96:PHE:CD1	28:Aj:170:LEU:HG	2.56	0.41
14:AQ:16:LYS:N	14:AQ:29:ARG:O	2.51	0.41
14:AQ:85:ILE:HG23	21:Ac:77:ARG:NH1	2.34	0.41
23:Ae:120:UNK:HG1	23:Ae:123:UNK:CG	2.50	0.41
23:Ae:243:UNK:HA	28:Aj:146:GLU:HG3	2.01	0.41
23:Ae:386:UNK:HA	23:Ae:389:UNK:HG3	2.02	0.41
26:Ah:361:LYS:O	26:Ah:364:HIS:HB2	2.21	0.41
38:B2:93:ARG:HH12	70:Be:83:PRO:CA	2.33	0.41
39:B3:88:MET:HE2	39:B3:88:MET:HB3	1.94	0.41
42:B6:20:MET:HE2	42:B6:20:MET:HB3	1.86	0.41
46:BA:163:A:H4'	46:BA:164:A:O4'	2.20	0.41
46:BA:518:C:O2'	53:BK:103:HIS:HE1	2.03	0.41
46:BA:1144:G:H1'	46:BA:1248:A:C2	2.55	0.41
48:BD:72:TYR:OH	48:BD:106:MET:O	2.30	0.41
50:BF:279:ARG:NH1	50:BF:282:PRO:HD3	2.34	0.41
57:BQ:163:MET:HE2	57:BQ:163:MET:HB3	1.78	0.41
58:BR:65:LEU:HD23	58:BR:65:LEU:HA	1.73	0.41
58:BR:91:GLN:O	58:BR:95:PRO:HG2	2.20	0.41
60:BT:288:ALA:HA	60:BT:291:ASN:HD22	1.85	0.41
62:BV:98:ARG:HD3	62:BV:113:THR:HG21	2.03	0.41
63:BW:104:LEU:HD11	63:BW:115:ILE:HG22	2.01	0.41
66:Ba:140:ALA:HB2	66:Ba:416:ALA:HB2	2.01	0.41
66:Ba:202:ILE:HA	66:Ba:202:ILE:HD13	1.82	0.41
67:Bb:153:GLU:HG2	67:Bb:158:TYR:CD2	2.54	0.41
70:Be:134:PRO:O	70:Be:135:ARG:HG3	2.20	0.41
73:Bh:59:ARG:HA	73:Bh:184:PHE:CE1	2.55	0.41
74:Bi:213:THR:HG21	74:Bi:245:TYR:CZ	2.56	0.41
75:Bj:182:GLU:OE1	75:Bj:187:THR:OG1	2.38	0.41
77:Bl:57:ILE:HA	77:Bl:58:PRO:HD2	1.88	0.41
81:Bp:8:LEU:HB3	81:Bp:95:GLN:CD	2.45	0.41
86:Bw:251:ILE:HA	86:Bw:252:PRO:HD2	1.86	0.41
86:Bw:419:LEU:HA	86:Bw:419:LEU:HD12	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
87:Bx:100:LEU:HA	87:Bx:100:LEU:HD12	1.70	0.41
1:AA:162:C:H5"	1:AA:163:A:N7	2.36	0.41
5:AF:114:GLU:HG2	5:AF:117:LEU:HD21	2.01	0.41
8:AJ:70:ASP:HB2	32:Ao:61:LYS:C	2.45	0.41
10:AL:49:MET:HE2	10:AL:49:MET:HB3	1.90	0.41
17:AV:43:Y5P:H2'	17:AV:44:Y5P:C6	2.50	0.41
19:Aa:342:UNK:CA	19:Aa:345:UNK:HG3	2.48	0.41
21:Ac:3:MET:HB3	21:Ac:3:MET:HE2	1.69	0.41
22:Ad:44:THR:HA	22:Ad:45:PRO:HD3	1.84	0.41
22:Ad:49:ASP:O	22:Ad:53:PHE:HB2	2.21	0.41
25:Ag:210:ASN:ND2	25:Ag:231:ARG:NH1	2.68	0.41
25:Ag:365:LEU:HD23	25:Ag:370:ALA:HB1	2.01	0.41
27:Ai:18:LEU:HD23	29:Ak:231:LEU:HD23	2.02	0.41
29:Ak:85:LEU:H	29:Ak:85:LEU:HG	1.60	0.41
32:Ao:654:UNK:C	32:Ao:657:UNK:HG3	2.51	0.41
33:Ap:179:THR:CG2	33:Ap:184:VAL:HG11	2.50	0.41
40:B4:64:THR:OG1	69:Bd:178:TYR:HB3	2.20	0.41
46:BA:138:G:C6	74:Bi:72:LEU:HB3	2.55	0.41
46:BA:442:G:N2	46:BA:445:C:H3'	2.35	0.41
46:BA:473:A:O2'	46:BA:474:C:P	2.78	0.41
46:BA:856:U:O2'	48:BD:67:LYS:NZ	2.53	0.41
46:BA:1180:G:H4'	46:BA:1228:U:O2'	2.19	0.41
49:BE:227:GLN:CD	49:BE:227:GLN:N	2.79	0.41
52:BJ:89:VAL:O	52:BJ:93:ASN:ND2	2.53	0.41
55:BO:138:LEU:HA	55:BO:138:LEU:HD12	1.78	0.41
60:BT:68:UNK:O	60:BT:68:UNK:CG	2.68	0.41
60:BT:96:ARG:NH1	60:BT:285:GLU:CD	2.77	0.41
61:BU:116:LEU:O	61:BU:119:LEU:HB3	2.20	0.41
62:BV:119:LEU:HD11	62:BV:194:GLN:HB3	2.01	0.41
62:BV:139:LEU:HD13	62:BV:148:LEU:CD2	2.49	0.41
63:BW:198:ILE:HD11	71:Bf:116:PHE:CE1	2.56	0.41
66:Ba:413:LYS:O	66:Ba:416:ALA:HB3	2.20	0.41
67:Bb:41:ASP:O	67:Bb:48:LEU:HD11	2.20	0.41
68:Bc:153:ARG:NH1	68:Bc:256:ASP:HB2	2.35	0.41
68:Bc:313:LEU:HD12	68:Bc:313:LEU:HA	1.80	0.41
70:Be:44:ARG:NH1	86:Bw:158:PRO:HD3	2.36	0.41
74:Bi:80:CYS:SG	74:Bi:166:GLU:HG2	2.61	0.41
86:Bw:371:LEU:HD12	86:Bw:371:LEU:HA	1.73	0.41
87:Bx:54:THR:HG22	87:Bx:55:GLU:H	1.85	0.41
1:AA:128:C:H2'	1:AA:129:G:O4'	2.20	0.41
1:AA:228:G:H2'	1:AA:229:U:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:630:A:H2	1:AA:654:A:N6	2.19	0.41
1:AA:746:A:H2'	1:AA:747:C:O4'	2.20	0.41
1:AA:916:A:H2'	1:AA:917:C:C1'	2.51	0.41
7:AI:88:LEU:HD11	7:AI:107:ALA:HB1	2.02	0.41
10:AL:39:LEU:HD22	10:AL:39:LEU:HA	1.73	0.41
13:AP:20:ARG:HA	13:AP:87:VAL:HG21	2.02	0.41
14:AQ:96:THR:HB	14:AQ:98:LYS:HZ3	1.82	0.41
15:AR:57:ASN:HA	15:AR:58:PRO:HD3	1.74	0.41
16:AU:59:THR:O	16:AU:63:ILE:HG13	2.20	0.41
17:AY:55:Y5P:C6	17:AY:57:Y5P:H5	2.44	0.41
25:Ag:116:PHE:HB3	25:Ag:302:GLY:HA2	2.02	0.41
25:Ag:382:LEU:HB3	25:Ag:393:LEU:CD1	2.50	0.41
32:Ao:86:PRO:HG2	32:Ao:89:PHE:HD2	1.86	0.41
32:Ao:225:UNK:HG1	32:Ao:263:UNK:CB	2.46	0.41
32:Ao:411:UNK:HA	32:Ao:414:UNK:HG3	2.02	0.41
37:B1:163:ARG:NH2	66:Ba:55:LEU:HD21	2.35	0.41
37:B1:190:ARG:H	37:B1:190:ARG:HG2	1.69	0.41
37:B1:201:ALA:O	37:B1:204:VAL:HG12	2.21	0.41
38:B2:126:LEU:HD12	38:B2:126:LEU:HA	1.74	0.41
38:B2:221:ILE:H	38:B2:221:ILE:HG13	1.72	0.41
46:BA:214:A:P	50:BF:92:ARG:HH22	2.43	0.41
46:BA:219:G:N3	46:BA:230:C:O2'	2.53	0.41
46:BA:553:C:C4'	87:Bx:102:ARG:HH12	2.33	0.41
46:BA:870:A:H5"	46:BA:871:U:OP2	2.20	0.41
46:BA:1081:C:H2'	46:BA:1082:C:C6	2.55	0.41
46:BA:1129:U:H2'	46:BA:1130:G:C8	2.56	0.41
47:BB:33:Y5P:H2'	47:BB:34:Y5P:HA1	2.03	0.41
47:BB:65:Y5P:H2'	47:BB:66:P5P:C8	2.33	0.41
54:BN:112:LEU:HD23	54:BN:112:LEU:HA	1.76	0.41
55:BO:52:HIS:HD2	55:BO:53:ARG:HG3	1.86	0.41
56:BP:100:ARG:O	56:BP:103:TYR:HB3	2.21	0.41
56:BP:178:PHE:HB2	56:BP:214:TYR:CE2	2.55	0.41
58:BR:64:LYS:HE2	58:BR:97:PHE:O	2.21	0.41
59:BS:74:SER:HB3	59:BS:147:HIS:HE1	1.85	0.41
60:BT:117:LEU:HD22	60:BT:176:VAL:HG22	2.02	0.41
61:BU:64:LEU:HD22	61:BU:64:LEU:HA	1.58	0.41
65:BY:159:PHE:CG	65:BY:160:PRO:HD2	2.56	0.41
68:Bc:211:LEU:HA	68:Bc:212:PRO:HD3	1.81	0.41
72:Bg:28:ARG:HH11	72:Bg:28:ARG:CB	2.34	0.41
73:Bh:196:PHE:O	73:Bh:199:ILE:HB	2.20	0.41
75:Bj:72:ASP:O	75:Bj:75:GLN:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:Bj:148:SER:OG	75:Bj:151:ARG:HB2	2.20	0.41
77:Bl:77:ASP:OD1	77:Bl:77:ASP:N	2.53	0.41
79:Bn:75:LYS:HA	79:Bn:81:ARG:HH12	1.85	0.41
87:Bx:118:CYS:SG	87:Bx:181:LEU:HD11	2.60	0.41
1:AA:65:C:OP2	22:Ad:30:ARG:HB2	2.21	0.41
1:AA:246:A:H2'	1:AA:247:G:O4'	2.21	0.41
1:AA:677:C:H2'	1:AA:678:G:O4'	2.21	0.41
1:AA:823:G:H5'	1:AA:824:G:OP2	2.21	0.41
3:AC:73:THR:HG21	29:Ak:160:SER:HB3	2.02	0.41
7:AI:389:ARG:HA	7:AI:389:ARG:HD3	1.89	0.41
12:AO:68:PRO:HA	12:AO:69:PRO:HD3	1.80	0.41
16:AU:68:MET:O	16:AU:72:ILE:HG12	2.20	0.41
17:AV:53:Y5P:O5'	17:AV:53:Y5P:H6	2.19	0.41
17:AY:32:Y5P:H4A	17:AY:33:Y5P:C4	2.40	0.41
17:AY:62:Y5P:N3	17:AY:63:Y5P:H4	2.35	0.41
19:Aa:282:GLY:O	19:Aa:286:ASP:HB2	2.21	0.41
19:Aa:310:UNK:HG3	19:Aa:313:UNK:HB2	2.03	0.41
19:Aa:310:UNK:HG2	19:Aa:313:UNK:HG2	1.93	0.41
22:Ad:151:GLN:O	22:Ad:155:GLN:HG3	2.21	0.41
23:Ae:244:UNK:O	23:Ae:244:UNK:HG2	2.20	0.41
23:Ae:246:UNK:O	23:Ae:247:UNK:CG	2.67	0.41
26:Ah:286:PHE:HD1	26:Ah:291:GLU:HG3	1.86	0.41
29:Ak:212:ASP:O	29:Ak:214:CYS:N	2.53	0.41
32:Ao:123:SER:O	32:Ao:125:PRO:HD3	2.19	0.41
32:Ao:398:UNK:O	32:Ao:401:UNK:HG3	2.20	0.41
32:Ao:514:UNK:CB	32:Ao:541:UNK:HG1	2.48	0.41
32:Ao:538:UNK:O	32:Ao:542:UNK:HG3	2.21	0.41
38:B2:72:ASP:HA	38:B2:73:PRO:HD3	1.95	0.41
38:B2:156:ARG:CA	70:Be:128:LEU:HD13	2.50	0.41
46:BA:48:U:O2'	46:BA:49:A:H4'	2.20	0.41
46:BA:529:G:H1	46:BA:544:C:N4	2.13	0.41
46:BA:672:U:O5'	46:BA:672:U:H6	2.04	0.41
46:BA:680:G:H1	46:BA:695:C:H42	1.69	0.41
46:BA:1452:C:H2'	46:BA:1453:C:O4'	2.21	0.41
48:BD:82:SER:O	48:BD:82:SER:OG	2.34	0.41
56:BP:56:GLU:HG2	56:BP:62:ARG:CA	2.49	0.41
56:BP:61:THR:O	56:BP:62:ARG:C	2.64	0.41
56:BP:160:SER:O	56:BP:164:ILE:HG13	2.21	0.41
67:Bb:237:VAL:HG21	67:Bb:240:ILE:HD11	2.01	0.41
68:Bc:276:GLU:HG2	68:Bc:309:TRP:HZ2	1.86	0.41
75:Bj:64:THR:HG22	75:Bj:66:LEU:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:Bk:53:THR:O	76:Bk:56:ILE:HG12	2.21	0.41
77:Bl:108:THR:OG1	77:Bl:151:GLY:O	2.38	0.41
86:Bw:158:PRO:HB2	86:Bw:160:ILE:HG22	2.02	0.41
88:Bz:21:UNK:CA	88:Bz:24:UNK:HG3	2.46	0.41
88:Bz:34:UNK:CG	88:Bz:35:UNK:N	2.83	0.41
1:AA:559:U:H3	1:AA:712:A:H61	1.68	0.41
1:AA:925:A:O2'	1:AA:946:A:H5'	2.21	0.41
6:AG:154:PRO:HG3	6:AG:186:TRP:CH2	2.56	0.41
7:AI:201:LEU:HB3	7:AI:205:GLU:HB2	2.03	0.41
8:AJ:179:GLN:HG3	8:AJ:180:LEU:H	1.85	0.41
9:AK:135:ILE:HD11	9:AK:169:MET:HE3	2.02	0.41
9:AK:176:SER:HB2	16:AU:13:MET:HG2	2.02	0.41
12:AO:69:PRO:HA	12:AO:70:PRO:HD3	1.84	0.41
12:AO:223:LYS:HB2	12:AO:223:LYS:HE3	1.81	0.41
13:AP:59:ASN:OD1	13:AP:63:GLU:N	2.47	0.41
14:AQ:8:VAL:C	14:AQ:10:ALA:H	2.28	0.41
17:AY:61:Y5P:H4A	17:AY:62:Y5P:H4	2.02	0.41
19:Aa:90:PHE:CE2	19:Aa:121:ALA:HB2	2.55	0.41
19:Aa:350:UNK:HA	19:Aa:353:UNK:HG3	2.03	0.41
21:Ac:75:PHE:CE2	21:Ac:77:ARG:HG3	2.55	0.41
23:Ae:32:UNK:O	23:Ae:36:UNK:HB1	2.21	0.41
24:Af:136:GLN:H	24:Af:139:THR:CB	2.33	0.41
25:Ag:154:ILE:HG13	25:Ag:186:TRP:HE1	1.84	0.41
25:Ag:191:LYS:HZ2	25:Ag:222:GLY:HA2	1.86	0.41
25:Ag:202:LYS:HD3	25:Ag:202:LYS:HA	1.83	0.41
25:Ag:350:LYS:HG3	25:Ag:351:GLU:N	2.36	0.41
31:An:136:ARG:O	31:An:140:HIS:N	2.52	0.41
37:B1:42:HIS:HE1	37:B1:84:GLY:H	1.68	0.41
37:B1:173:ASP:HB3	37:B1:175:GLN:HG2	2.01	0.41
37:B1:226:LEU:HB2	38:B2:158:LEU:HD12	2.02	0.41
44:B8:103:LYS:NZ	46:BA:76:G:P	2.93	0.41
46:BA:69:C:N4	85:Bv:49:ARG:NH1	2.68	0.41
46:BA:288:U:O2'	46:BA:289:A:H5'	2.21	0.41
46:BA:441:G:OP1	57:BQ:144:LYS:HE3	2.20	0.41
46:BA:1021:U:H2'	46:BA:1022:G:C8	2.54	0.41
48:BD:128:ILE:HD11	48:BD:144:ALA:CB	2.50	0.41
54:BN:81:THR:HB	54:BN:83:TYR:CD2	2.52	0.41
57:BQ:185:PHE:CD1	57:BQ:185:PHE:N	2.87	0.41
58:BR:59:LEU:N	60:BT:269:MET:HE1	2.36	0.41
62:BV:136:LYS:CE	80:Bo:48:ASP:HB3	2.51	0.41
65:BY:133:VAL:CG1	65:BY:145:ARG:HB3	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:BY:212:LYS:NZ	65:BY:214:TYR:CE1	2.85	0.41
66:Ba:230:LEU:O	66:Ba:289:HIS:HB3	2.21	0.41
66:Ba:237:PRO:HA	66:Ba:238:PRO:HD2	1.91	0.41
67:Bb:106:ARG:O	67:Bb:110:LEU:HG	2.20	0.41
67:Bb:235:TRP:HB2	67:Bb:254:TYR:HA	2.02	0.41
68:Bc:140:TRP:NE1	68:Bc:171:VAL:HA	2.24	0.41
69:Bd:89:ILE:H	69:Bd:89:ILE:HG13	1.57	0.41
73:Bh:81:GLU:HB2	73:Bh:83:PHE:HE1	1.86	0.41
74:Bi:180:THR:HB	74:Bi:225:TYR:HB2	2.01	0.41
85:Bv:146:UNK:HA	85:Bv:149:UNK:HG3	2.03	0.41
88:Bz:9:UNK:O	88:Bz:12:UNK:HG3	2.21	0.41
1:AA:57:A:P	1:AA:203:G:H21	2.43	0.41
1:AA:124:A:H1'	1:AA:125:U:H5	1.84	0.41
1:AA:221:A:P	33:Ap:148:LYS:NZ	2.93	0.41
1:AA:875:A:N6	28:Aj:17:ARG:HH11	2.18	0.41
6:AG:153:GLU:HG3	6:AG:179:ARG:HB3	2.03	0.41
8:AJ:165:PRO:HB2	8:AJ:168:VAL:HG22	2.02	0.41
11:AN:71:ALA:O	11:AN:75:ILE:HG12	2.21	0.41
12:AO:113:MET:HE3	12:AO:128:ALA:HB1	2.03	0.41
12:AO:210:LEU:HD11	31:An:177:TRP:HE1	1.85	0.41
17:AV:53:Y5P:H2'	17:AV:54:Y5P:H6	2.01	0.41
17:AY:54:Y5P:H4A	17:AY:55:Y5P:C4	2.47	0.41
20:Ab:75:TYR:CZ	24:Af:99:LYS:NZ	2.89	0.41
21:Ac:137:ARG:NH2	21:Ac:143:VAL:HG22	2.35	0.41
23:Ae:28:UNK:HB1	23:Ae:369:UNK:CG	2.51	0.41
23:Ae:118:UNK:C	23:Ae:119:UNK:CG	2.98	0.41
23:Ae:221:UNK:O	23:Ae:225:UNK:HB1	2.21	0.41
23:Ae:223:UNK:O	23:Ae:226:UNK:CG	2.69	0.41
32:Ao:225:UNK:O	32:Ao:266:UNK:HG1	2.20	0.41
32:Ao:307:UNK:HB2	32:Ao:343:UNK:HG2	2.02	0.41
32:Ao:550:UNK:CA	32:Ao:553:UNK:HG3	2.45	0.41
33:Ap:193:LEU:HD23	33:Ap:193:LEU:HA	1.89	0.41
37:B1:37:THR:HA	37:B1:38:PRO:HD2	1.91	0.41
39:B3:89:LEU:HD23	39:B3:89:LEU:HA	1.79	0.41
39:B3:148:ARG:NH2	39:B3:151:LEU:HD22	2.35	0.41
46:BA:192:U:H2'	46:BA:193:G:H8	1.86	0.41
46:BA:1159:G:H4'	46:BA:1227:A:H5'	2.02	0.41
49:BE:104:LEU:HB2	49:BE:121:LEU:O	2.21	0.41
49:BE:243:ILE:H	49:BE:243:ILE:HG12	1.70	0.41
60:BT:103:ARG:NE	60:BT:108:ILE:HD12	2.36	0.41
60:BT:194:LEU:HA	60:BT:195:PRO:HD3	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:BX:77:ASN:HD22	64:BX:77:ASN:HA	1.61	0.41
64:BX:144:VAL:HA	64:BX:145:PRO:HD3	1.79	0.41
65:BY:73:GLN:NE2	65:BY:128:ARG:O	2.54	0.41
68:Bc:77:VAL:O	74:Bi:279:THR:HG23	2.20	0.41
75:Bj:198:ASN:HD21	75:Bj:200:MET:HB3	1.86	0.41
82:Bq:107:LEU:HD13	82:Bq:120:LEU:HD12	2.03	0.41
86:Bw:86:MET:HB3	86:Bw:88:PHE:CE2	2.55	0.41
86:Bw:171:LEU:HD23	86:Bw:232:HIS:CD2	2.56	0.41
1:AA:190:G:H21	1:AA:192:C:N4	2.19	0.41
1:AA:345:U:O4	9:AK:122:ALA:HA	2.21	0.41
1:AA:387:C:H5"	5:AF:95:LYS:HG3	2.03	0.41
1:AA:687:A:O2'	11:AN:96:ARG:HB2	2.21	0.41
1:AA:805:G:H2'	1:AA:806:A:O4'	2.21	0.41
1:AA:873:A:O2'	1:AA:874:U:H5'	2.20	0.41
1:AA:942:G:N1	1:AA:945:A:OP2	2.54	0.41
2:AB:174:LEU:HA	2:AB:174:LEU:HD12	1.64	0.41
4:AE:198:TRP:O	4:AE:222:ILE:HB	2.21	0.41
4:AE:255:GLY:N	4:AE:279:LEU:HD23	2.36	0.41
4:AE:289:THR:HG22	4:AE:290:ILE:H	1.85	0.41
5:AF:2:PRO:HB2	5:AF:96:HIS:CG	2.56	0.41
6:AG:112:THR:HG23	25:Ag:396:TYR:HB3	2.03	0.41
7:AI:397:ARG:HE	17:AV:33:Y5P:H5	1.86	0.41
13:AP:111:ARG:NH2	19:Aa:146:ILE:HA	2.36	0.41
16:AU:25:THR:O	16:AU:29:ILE:HG12	2.21	0.41
17:AV:25:Y5P:H4A	17:AV:26:Y5P:H4	2.01	0.41
19:Aa:141:LEU:HD21	19:Aa:182:LYS:HE3	2.02	0.41
19:Aa:167:ARG:NH1	19:Aa:185:TRP:CH2	2.89	0.41
19:Aa:310:UNK:HG1	19:Aa:313:UNK:HG2	1.91	0.41
19:Aa:347:UNK:HG2	19:Aa:348:UNK:N	2.35	0.41
21:Ac:56:GLN:NE2	21:Ac:64:ILE:HB	2.36	0.41
22:Ad:55:VAL:O	22:Ad:59:ARG:HG3	2.20	0.41
23:Ae:172:UNK:O	23:Ae:177:UNK:HG1	2.21	0.41
23:Ae:215:UNK:HA	23:Ae:218:UNK:HG3	2.03	0.41
25:Ag:69:UNK:HG2	25:Ag:74:LEU:HD13	2.03	0.41
25:Ag:77:VAL:C	25:Ag:79:PRO:HD3	2.46	0.41
25:Ag:89:GLN:CD	25:Ag:93:PHE:HE2	2.29	0.41
25:Ag:101:ARG:HB3	25:Ag:103:PRO:HD2	2.02	0.41
25:Ag:123:TYR:HE1	25:Ag:340:ILE:HD12	1.86	0.41
26:Ah:286:PHE:CD1	26:Ah:291:GLU:HG3	2.55	0.41
26:Ah:339:ILE:HD11	26:Ah:386:LEU:HD13	2.03	0.41
28:Aj:114:ALA:C	28:Aj:131:ILE:HG13	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Ak:199:ARG:HG2	29:Ak:199:ARG:NH1	2.36	0.41
30:Am:6:LEU:HD13	30:Am:6:LEU:HA	1.85	0.41
32:Ao:339:UNK:HG2	32:Ao:376:UNK:CB	2.23	0.41
32:Ao:423:UNK:HB2	32:Ao:440:UNK:HG2	2.03	0.41
32:Ao:423:UNK:O	32:Ao:427:UNK:HG3	2.21	0.41
32:Ao:486:UNK:O	32:Ao:490:UNK:HG1	2.19	0.41
32:Ao:532:UNK:HA	32:Ao:535:UNK:HG3	2.03	0.41
36:B0:76:HIS:O	36:B0:130:PHE:HA	2.21	0.41
36:B0:120:LEU:HA	36:B0:121:PRO:HD2	1.87	0.41
37:B1:16:LEU:O	37:B1:21:TYR:HB2	2.20	0.41
37:B1:43:TYR:HB3	37:B1:67:ILE:HD12	2.02	0.41
37:B1:119:LEU:HG	37:B1:165:MET:HE2	2.03	0.41
38:B2:93:ARG:NH1	70:Be:83:PRO:HA	2.35	0.41
38:B2:123:ARG:HH12	64:BX:30:ARG:CB	2.32	0.41
41:B5:94:ARG:O	63:BW:87:TYR:OH	2.27	0.41
41:B5:131:ARG:HD2	41:B5:131:ARG:HA	1.85	0.41
44:B8:116:ARG:HG3	44:B8:122:TRP:CE2	2.56	0.41
46:BA:242:A:C4	46:BA:350:A:C2	3.08	0.41
46:BA:251:G:C6	46:BA:320:A:C4	3.09	0.41
46:BA:356:U:H5"	46:BA:356:U:C6	2.55	0.41
46:BA:513:A:C8	46:BA:539:A:H4'	2.56	0.41
46:BA:532:A:H2'	46:BA:533:G:O4'	2.21	0.41
46:BA:632:G:H2'	46:BA:632:G:N3	2.36	0.41
46:BA:658:C:O3'	58:BR:81:THR:HG21	2.21	0.41
46:BA:658:C:C4'	58:BR:81:THR:HG21	2.47	0.41
46:BA:750:U:C2'	46:BA:751:G:H5'	2.51	0.41
46:BA:774:C:O2'	46:BA:775:A:H8	2.04	0.41
46:BA:812:C:O2	46:BA:812:C:H5'	2.21	0.41
46:BA:885:C:H5'	46:BA:886:A:OP2	2.21	0.41
46:BA:1015:U:O2'	46:BA:1438:U:H5'	2.20	0.41
46:BA:1198:A:H2'	46:BA:1200:C:OP2	2.21	0.41
46:BA:1293:G:O2'	46:BA:1299:A:N6	2.52	0.41
46:BA:1307:U:H2'	46:BA:1308:A:H8	1.86	0.41
47:BB:25:P5P:O5'	59:BS:86:THR:HG21	2.21	0.41
48:BD:288:ARG:HA	48:BD:289:PRO:HD2	1.93	0.41
49:BE:80:LEU:HD12	49:BE:80:LEU:HA	1.87	0.41
49:BE:98:GLY:HA3	49:BE:179:PHE:CE1	2.55	0.41
50:BF:191:ASP:C	50:BF:192:SER:HG	2.24	0.41
50:BF:205:GLU:HA	50:BF:208:ARG:HB2	2.03	0.41
50:BF:220:ASP:OD1	50:BF:221:LEU:N	2.54	0.41
50:BF:263:LEU:N	50:BF:264:PRO:HD2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:BK:94:ALA:HB1	53:BK:116:HIS:CD2	2.56	0.41
54:BN:116:LEU:HD23	54:BN:116:LEU:HA	1.66	0.41
54:BN:155:LEU:HB2	87:Bx:86:VAL:HG11	2.02	0.41
54:BN:178:LEU:HD12	87:Bx:35:PHE:CD1	2.56	0.41
55:BO:95:ARG:HA	55:BO:95:ARG:HH11	1.85	0.41
58:BR:84:ASP:O	58:BR:87:PRO:HD2	2.21	0.41
60:BT:76:LEU:HB2	60:BT:283:TRP:HZ3	1.85	0.41
60:BT:185:ASN:OD1	60:BT:185:ASN:N	2.54	0.41
61:BU:68:TRP:CZ2	61:BU:100:LYS:HB2	2.56	0.41
66:Ba:163:LEU:HD23	66:Ba:163:LEU:HA	1.79	0.41
67:Bb:255:LEU:HA	67:Bb:256:PRO:HD3	1.93	0.41
68:Bc:166:ALA:HA	68:Bc:167:PRO:HD2	1.95	0.41
68:Bc:211:LEU:O	68:Bc:269:THR:OG1	2.27	0.41
69:Bd:143:GLN:HE22	75:Bj:210:CYS:HA	1.85	0.41
69:Bd:165:ASP:OD2	69:Bd:167:SER:HB2	2.21	0.41
71:Bf:135:LYS:HA	71:Bf:136:PRO:HD3	1.82	0.41
72:Bg:55:ALA:HB1	78:Bm:152:ASN:OD1	2.21	0.41
73:Bh:301:LEU:HD12	73:Bh:301:LEU:HA	1.74	0.41
74:Bi:129:ASP:HA	74:Bi:130:PRO:HD2	1.94	0.41
78:Bm:54:PRO:HA	78:Bm:55:PRO:HD3	1.87	0.41
85:Bv:127:LYS:HE3	85:Bv:131:MET:HG3	2.03	0.41
86:Bw:49:ALA:O	86:Bw:61:ARG:HD3	2.21	0.41
86:Bw:258:MET:HE2	86:Bw:258:MET:HB3	1.93	0.41
86:Bw:363:PHE:HB2	86:Bw:390:THR:OG1	2.21	0.41
87:Bx:151:LEU:HD23	87:Bx:151:LEU:HA	1.77	0.41
88:Bz:30:UNK:HA	88:Bz:33:UNK:HG3	2.03	0.41
88:Bz:610:UNK:HA	88:Bz:613:UNK:CG	2.46	0.41
1:AA:308:A:H8	1:AA:308:A:OP2	2.03	0.41
1:AA:475:A:P	5:AF:123:ARG:HH22	2.42	0.41
1:AA:540:U:H1'	1:AA:541:C:H5	1.86	0.41
1:AA:679:U:H2'	1:AA:680:U:C6	2.56	0.41
1:AA:816:U:H5"	7:AI:339:SER:HB2	2.03	0.41
4:AE:206:PRO:HA	4:AE:272:LYS:HD2	2.03	0.41
4:AE:270:LYS:O	4:AE:274:ARG:HB2	2.21	0.41
5:AF:58:HIS:CD2	5:AF:89:ILE:HD11	2.56	0.41
5:AF:63:TYR:OH	15:AR:119:GLY:O	2.37	0.41
6:AG:223:LYS:O	6:AG:226:MET:HB3	2.20	0.41
7:AI:71:VAL:HG12	7:AI:75:LYS:HE3	2.03	0.41
7:AI:90:ASN:ND2	29:Ak:65:ASP:O	2.54	0.41
12:AO:67:ASP:O	12:AO:69:PRO:HD3	2.21	0.41
12:AO:96:LEU:HD13	12:AO:104:LYS:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AQ:98:LYS:HE3	14:AQ:109:PRO:HG3	2.03	0.41
17:AV:21:Y5P:HC	17:AV:48:Y5P:H4	2.03	0.41
17:AY:8:Y5P:C4	17:AY:14:Y5P:H5	2.51	0.41
23:Ae:211:UNK:HA	23:Ae:216:UNK:HG1	2.02	0.41
23:Ae:224:UNK:HA	23:Ae:227:UNK:HG3	2.01	0.41
23:Ae:250:UNK:O	23:Ae:254:UNK:HG3	2.21	0.41
26:Ah:348:CYS:SG	26:Ah:352:LYS:HE3	2.61	0.41
32:Ao:193:UNK:HG2	32:Ao:227:UNK:HB2	2.02	0.41
32:Ao:346:UNK:HA	32:Ao:349:UNK:HG3	2.03	0.41
32:Ao:396:UNK:CA	32:Ao:399:UNK:HG3	2.51	0.41
41:B5:178:GLU:OE1	41:B5:178:GLU:N	2.54	0.41
46:BA:438:A:H2'	46:BA:439:A:H5"	2.02	0.41
46:BA:470:U:C4	46:BA:471:U:C4	3.09	0.41
46:BA:750:U:O2'	46:BA:751:G:H5'	2.21	0.41
46:BA:1052:A:H5'	46:BA:1053:A:OP2	2.21	0.41
46:BA:1413:G:H2'	46:BA:1414:G:O4'	2.20	0.41
46:BA:1439:A:H2'	46:BA:1440:U:O4'	2.20	0.41
48:BD:73:THR:HG22	48:BD:75:MET:N	2.33	0.41
49:BE:82:ASP:O	49:BE:83:GLU:HG3	2.20	0.41
49:BE:95:SER:OG	49:BE:181:VAL:HA	2.20	0.41
53:BK:104:THR:HG23	53:BK:152:GLY:HA2	2.03	0.41
53:BK:124:LYS:HB3	53:BK:124:LYS:HE3	1.81	0.41
56:BP:247:ILE:H	56:BP:247:ILE:CD1	2.34	0.41
56:BP:255:MET:HE3	56:BP:255:MET:HB3	1.77	0.41
62:BV:63:PRO:HA	62:BV:64:PRO:HD3	1.76	0.41
64:BX:105:PHE:CG	64:BX:106:THR:N	2.89	0.41
66:Ba:85:PRO:HA	66:Ba:88:ARG:HH12	1.86	0.41
67:Bb:218:LEU:HD13	67:Bb:270:PHE:CE1	2.56	0.41
68:Bc:76:PHE:HE2	68:Bc:91:HIS:HB2	1.86	0.41
68:Bc:140:TRP:CE3	68:Bc:140:TRP:HA	2.56	0.41
71:Bf:69:TYR:CE1	73:Bh:256:ARG:NH1	2.89	0.41
73:Bh:199:ILE:HD11	73:Bh:214:PHE:CE1	2.56	0.41
74:Bi:174:TRP:HD1	74:Bi:175:ASP:OD2	2.05	0.41
75:Bj:139:GLU:O	75:Bj:143:LYS:N	2.32	0.41
86:Bw:83:LEU:HD23	86:Bw:83:LEU:HA	1.76	0.41
86:Bw:295:LEU:HD12	86:Bw:356:THR:O	2.21	0.41
87:Bx:165:LYS:HA	87:Bx:165:LYS:HD3	1.77	0.41
88:Bz:399:UNK:C	88:Bz:402:UNK:HG3	2.51	0.41
88:Bz:602:UNK:HA	88:Bz:605:UNK:HG3	2.01	0.41
1:AA:202:A:OP1	13:AP:102:MET:HE3	2.21	0.40
1:AA:285:C:O2'	1:AA:488:A:C2	2.72	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:358:U:OP1	9:AK:154:LYS:HD3	2.21	0.40
1:AA:365:A:H1'	1:AA:417:C:N3	2.36	0.40
1:AA:434:A:H2'	1:AA:435:C:H6	1.86	0.40
1:AA:817:G:O6	7:AI:278:LYS:NZ	2.45	0.40
2:AB:71:PHE:HE2	2:AB:262:LYS:HG2	1.85	0.40
2:AB:115:ILE:H	2:AB:115:ILE:HG12	1.74	0.40
2:AB:203:GLU:HG3	30:Am:114:LYS:HZ2	1.86	0.40
4:AE:140:LEU:HB3	4:AE:146:ILE:HD13	2.03	0.40
5:AF:42:LEU:HD12	5:AF:63:TYR:HB3	2.03	0.40
7:AI:276:LYS:CE	7:AI:281:LYS:HE2	2.51	0.40
7:AI:358:THR:HG23	7:AI:360:ASP:H	1.86	0.40
8:AJ:181:PRO:O	8:AJ:184:ILE:HG22	2.22	0.40
17:AY:31:Y5P:H4A	17:AY:32:Y5P:C4	2.48	0.40
20:Ab:29:PRO:HB2	20:Ab:31:TRP:CD1	2.56	0.40
25:Ag:162:LYS:HE2	25:Ag:315:LEU:HD21	2.03	0.40
25:Ag:333:PHE:CD2	29:Ak:302:LYS:HE2	2.54	0.40
29:Ak:91:TYR:CD1	29:Ak:92:PRO:HD2	2.56	0.40
29:Ak:194:LYS:NZ	29:Ak:245:LYS:HZ1	2.19	0.40
32:Ao:201:UNK:HG2	32:Ao:202:UNK:N	2.36	0.40
32:Ao:374:UNK:C	32:Ao:377:UNK:HG3	2.51	0.40
32:Ao:507:UNK:CG	32:Ao:541:UNK:HB1	2.50	0.40
39:B3:65:LYS:HG2	80:Bo:84:MET:HE3	2.04	0.40
41:B5:185:PHE:CE2	58:BR:132:PRO:HA	2.56	0.40
45:B9:88:TYR:CE1	45:B9:96:LYS:HE2	2.56	0.40
46:BA:270:U:H5'	46:BA:271:A:OP2	2.21	0.40
46:BA:297:A:O4'	63:BW:159:ARG:HA	2.21	0.40
46:BA:568:A:H2'	46:BA:569:A:C8	2.57	0.40
46:BA:570:A:N6	46:BA:571:A:C6	2.89	0.40
46:BA:598:C:O2'	46:BA:599:C:H5'	2.21	0.40
46:BA:801:A:N6	46:BA:809:A:H61	2.20	0.40
46:BA:805:C:N4	46:BA:806:G:C6	2.89	0.40
46:BA:1130:G:C6	46:BA:1131:G:C5	3.08	0.40
46:BA:1393:A:OP2	46:BA:1393:A:H8	2.04	0.40
46:BA:1423:A:H4'	46:BA:1424:G:H5'	2.04	0.40
47:BB:43:Y5P:C2'	47:BB:44:Y5P:HA1	2.50	0.40
48:BD:188:LEU:HD23	48:BD:188:LEU:HA	1.79	0.40
50:BF:65:TRP:HZ3	78:Bm:99:PHE:HD1	1.69	0.40
53:BK:124:LYS:HB3	53:BK:124:LYS:HZ2	1.86	0.40
54:BN:71:LYS:HA	87:Bx:174:MET:HE2	2.03	0.40
56:BP:233:ARG:NH1	84:Bu:59:TRP:HZ3	2.20	0.40
58:BR:150:LEU:HD23	58:BR:150:LEU:HA	1.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:BR:153:LEU:HD23	58:BR:153:LEU:HA	1.86	0.40
59:BS:78:TRP:N	59:BS:174:GLU:OE1	2.43	0.40
60:BT:74:ARG:HD3	60:BT:283:TRP:CE2	2.56	0.40
62:BV:147:LEU:HD23	62:BV:147:LEU:HA	1.76	0.40
66:Ba:136:VAL:HG12	66:Ba:416:ALA:HB1	2.03	0.40
67:Bb:346:ARG:HA	67:Bb:347:PRO:HD3	1.95	0.40
75:Bj:217:PHE:HB2	75:Bj:227:LEU:HB3	2.03	0.40
77:Bl:85:PHE:HA	77:Bl:166:PHE:CE1	2.56	0.40
86:Bw:100:LEU:HD22	86:Bw:100:LEU:HA	1.68	0.40
86:Bw:250:SER:C	86:Bw:251:ILE:HG13	2.46	0.40
86:Bw:336:TYR:HD1	86:Bw:336:TYR:HA	1.75	0.40
87:Bx:108:CYS:O	87:Bx:111:GLU:N	2.54	0.40
87:Bx:192:LEU:HD23	87:Bx:192:LEU:HA	1.80	0.40
1:AA:586:U:H4'	11:AN:88:ARG:HG2	2.03	0.40
4:AE:261:ALA:HB2	4:AE:270:LYS:HZ2	1.86	0.40
6:AG:170:VAL:HA	6:AG:171:PRO:HD3	1.93	0.40
7:AI:100:THR:O	7:AI:104:ILE:HG13	2.22	0.40
8:AJ:122:LYS:HA	8:AJ:132:VAL:HG23	2.03	0.40
9:AK:177:ILE:HD11	16:AU:19:VAL:HG13	2.03	0.40
11:AN:67:LEU:HD23	11:AN:67:LEU:HA	1.91	0.40
12:AO:126:LEU:HB2	12:AO:171:LEU:HD21	2.02	0.40
21:Ac:125:HIS:HD2	21:Ac:127:ALA:HB3	1.87	0.40
22:Ad:143:ALA:O	22:Ad:147:GLN:HG3	2.21	0.40
23:Ae:219:UNK:CA	23:Ae:222:UNK:HG3	2.50	0.40
25:Ag:53:UNK:O	25:Ag:53:UNK:HG2	2.20	0.40
25:Ag:54:UNK:HG1	25:Ag:67:UNK:CA	2.47	0.40
25:Ag:64:UNK:O	25:Ag:64:UNK:HG2	2.20	0.40
25:Ag:104:ALA:O	25:Ag:108:LEU:HB2	2.20	0.40
26:Ah:308:ASN:OD1	26:Ah:311:ALA:HB2	2.21	0.40
32:Ao:487:UNK:HG2	32:Ao:488:UNK:N	2.36	0.40
36:B0:56:MET:N	36:B0:59:HIS:HD2	2.18	0.40
36:B0:79:ALA:HB2	67:Bb:74:TYR:HE2	1.86	0.40
36:B0:102:GLU:HB2	36:B0:130:PHE:CD2	2.56	0.40
37:B1:139:CYS:SG	51:BI:133:SER:HB2	2.61	0.40
41:B5:87:ILE:HD13	41:B5:91:ARG:HG3	2.03	0.40
42:B6:36:ARG:NH1	46:BA:1184:U:P	2.94	0.40
44:B8:175:ASP:HB3	44:B8:178:GLN:HB2	2.03	0.40
46:BA:480:A:N3	80:Bo:36:ASN:ND2	2.66	0.40
46:BA:481:G:OP1	80:Bo:23:ALA:N	2.54	0.40
46:BA:494:C:C4	46:BA:554:A:C2	3.09	0.40
46:BA:1157:U:C6	46:BA:1249:C:C5	3.08	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:BA:1308:A:H2'	46:BA:1309:G:O4'	2.21	0.40
51:BI:118:VAL:HG13	51:BI:122:ARG:HD3	2.02	0.40
56:BP:233:ARG:HG2	56:BP:234:LEU:N	2.35	0.40
62:BV:139:LEU:HD13	62:BV:148:LEU:HG	2.02	0.40
63:BW:58:PRO:HA	63:BW:59:PRO:HD3	1.93	0.40
64:BX:15:PRO:HA	65:BY:208:ARG:HH11	1.86	0.40
66:Ba:67:MET:HE2	66:Ba:67:MET:HB3	1.64	0.40
66:Ba:121:LEU:HD22	66:Ba:126:THR:HB	2.03	0.40
66:Ba:283:TYR:HD1	86:Bw:150:PHE:CG	2.40	0.40
67:Bb:79:GLY:C	67:Bb:81:GLU:N	2.79	0.40
74:Bi:198:ARG:HD3	74:Bi:198:ARG:HA	1.87	0.40
75:Bj:50:ALA:HA	75:Bj:175:GLN:HA	2.02	0.40
80:Bo:53:ASP:HB2	80:Bo:55:ARG:HG3	2.02	0.40
88:Bz:15:UNK:O	88:Bz:19:UNK:HG3	2.21	0.40
88:Bz:31:UNK:HA	88:Bz:34:UNK:CG	2.51	0.40
3:AC:72:HIS:CD2	3:AC:74:GLY:H	2.35	0.40
4:AE:261:ALA:HB2	4:AE:270:LYS:HZ1	1.87	0.40
9:AK:85:ILE:O	9:AK:150:ARG:NE	2.54	0.40
17:AY:11:Y5P:H6	17:AY:11:Y5P:O5'	2.21	0.40
20:Ab:12:ILE:HB	20:Ab:31:TRP:HH2	1.86	0.40
21:Ac:71:THR:HG22	21:Ac:73:SER:H	1.85	0.40
25:Ag:135:LEU:HD12	25:Ag:135:LEU:HA	1.78	0.40
28:Aj:83:LYS:HE2	28:Aj:87:TRP:CE2	2.57	0.40
31:An:189:TRP:CD1	31:An:191:THR:HG1	2.39	0.40
32:Ao:395:UNK:O	32:Ao:398:UNK:HG3	2.20	0.40
32:Ao:460:UNK:O	32:Ao:464:UNK:HG3	2.21	0.40
33:Ap:116:ASP:O	33:Ap:123:LEU:HD11	2.21	0.40
46:BA:139:A:OP2	65:BY:94:HIS:NE2	2.55	0.40
46:BA:367:A:H2'	46:BA:367:A:N3	2.36	0.40
47:BB:13:Y5P:H4	47:BB:24:P5P:C2	2.51	0.40
48:BD:76:PRO:HB2	48:BD:103:ARG:HD2	2.02	0.40
49:BE:131:LYS:H	49:BE:146:THR:HB	1.87	0.40
49:BE:314:LEU:HD23	49:BE:314:LEU:HA	1.77	0.40
50:BF:65:TRP:CE3	50:BF:76:ARG:HB2	2.57	0.40
54:BN:102:ALA:O	54:BN:106:LEU:HG	2.20	0.40
55:BO:128:ARG:HH22	60:BT:126:ALA:HB2	1.86	0.40
56:BP:253:PHE:O	56:BP:257:SER:OG	2.40	0.40
59:BS:64:LYS:HD3	59:BS:76:GLU:HG3	2.02	0.40
59:BS:85:ARG:HB3	59:BS:120:ARG:HH12	1.86	0.40
61:BU:11:ARG:HH12	61:BU:13:ARG:HH11	1.70	0.40
67:Bb:258:PHE:HD1	67:Bb:258:PHE:N	2.17	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:Bg:58:ASN:HA	72:Bg:59:PRO:HD2	1.88	0.40
75:Bj:257:LYS:NZ	75:Bj:273:ARG:HB2	2.36	0.40
76:Bk:175:HIS:HA	76:Bk:178:LEU:HG	2.03	0.40
77:Bl:129:SER:N	77:Bl:130:PRO:HD2	2.37	0.40
79:Bn:32:PHE:C	79:Bn:32:PHE:HD1	2.29	0.40
83:Bt:23:ARG:HD2	87:Bx:169:TRP:HB3	2.01	0.40
86:Bw:131:LEU:HD11	86:Bw:420:LEU:HD21	2.03	0.40
88:Bz:10:UNK:O	88:Bz:14:UNK:HG3	2.21	0.40
88:Bz:19:UNK:HA	88:Bz:22:UNK:HG3	2.02	0.40
88:Bz:405:UNK:HA	88:Bz:408:UNK:CG	2.52	0.40
1:AA:210:U:O4	1:AA:211:A:N6	2.54	0.40
1:AA:527:G:C6	1:AA:528:C:C4	3.09	0.40
5:AF:13:MET:HE2	5:AF:17:GLU:HB2	2.04	0.40
6:AG:119:LYS:HZ1	25:Ag:397:LEU:C	2.30	0.40
7:AI:395:LYS:HB3	7:AI:395:LYS:HE3	1.95	0.40
9:AK:91:LYS:O	9:AK:97:THR:HA	2.21	0.40
10:AL:96:PRO:HD3	10:AL:124:THR:HG23	2.04	0.40
17:AV:27:Y5P:C4	17:AV:28:Y5P:H4	2.52	0.40
17:AV:63:Y5P:H2'	17:AV:64:Y5P:C6	2.51	0.40
19:Aa:343:UNK:HA	19:Aa:346:UNK:HG3	2.03	0.40
24:Af:88:SER:HA	24:Af:89:PRO:HD3	1.84	0.40
32:Ao:208:UNK:HA	32:Ao:211:UNK:HG3	2.03	0.40
32:Ao:464:UNK:O	32:Ao:467:UNK:HG3	2.22	0.40
37:B1:16:LEU:HD12	37:B1:21:TYR:CD2	2.56	0.40
41:B5:101:ILE:HD11	63:BW:87:TYR:HB3	2.02	0.40
42:B6:55:LEU:HD23	85:Bv:131:MET:HB3	2.03	0.40
44:B8:157:LEU:HD11	44:B8:161:MET:HE2	2.03	0.40
45:B9:71:LYS:HE2	45:B9:77:TYR:HA	2.03	0.40
46:BA:242:A:C5	46:BA:350:A:C2	3.08	0.40
46:BA:428:G:C5'	56:BP:57:ARG:HD2	2.52	0.40
46:BA:993:C:H2'	46:BA:994:U:C6	2.56	0.40
46:BA:1291:G:O6	46:BA:1297:C:O2'	2.35	0.40
49:BE:177:LYS:HB3	49:BE:298:LYS:HD2	2.02	0.40
50:BF:248:LEU:HG	50:BF:253:MET:HE2	2.03	0.40
52:BJ:81:LEU:HD11	82:Bq:114:THR:C	2.45	0.40
52:BJ:90:PHE:CD1	52:BJ:96:ILE:HD13	2.57	0.40
54:BN:111:MET:HE2	54:BN:111:MET:HB3	1.59	0.40
56:BP:28:LYS:HE3	56:BP:29:PRO:O	2.21	0.40
58:BR:134:LEU:O	58:BR:136:LEU:N	2.55	0.40
63:BW:150:TYR:HB3	63:BW:166:GLU:HG2	2.03	0.40
63:BW:194:ALA:O	63:BW:198:ILE:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:BX:51:VAL:HG11	70:Be:55:ILE:HD13	2.04	0.40
66:Ba:302:ARG:NH1	66:Ba:302:ARG:HG3	2.36	0.40
66:Ba:336:LEU:HD23	66:Ba:336:LEU:HA	1.90	0.40
68:Bc:273:PHE:CD2	68:Bc:274:GLN:HG3	2.43	0.40
73:Bh:260:GLN:O	73:Bh:260:GLN:HG3	2.20	0.40
73:Bh:295:GLU:O	73:Bh:299:VAL:HG23	2.22	0.40
75:Bj:252:HIS:HD2	75:Bj:254:TRP:HE1	1.69	0.40
79:Bn:100:ASN:OD1	79:Bn:100:ASN:N	2.50	0.40
83:Bt:23:ARG:HA	83:Bt:24:PRO:HD2	1.84	0.40
86:Bw:206:ARG:HA	86:Bw:373:LEU:O	2.21	0.40
86:Bw:383:ARG:H	86:Bw:383:ARG:HG3	1.71	0.40
87:Bx:170:ASN:O	87:Bx:170:ASN:ND2	2.54	0.40
88:Bz:601:UNK:C	88:Bz:604:UNK:HG3	2.51	0.40
1:AA:39:A:N6	1:AA:40:A:C6	2.90	0.40
1:AA:95:A:H2'	1:AA:96:U:C6	2.57	0.40
1:AA:763:A:H4'	11:AN:75:ILE:HD12	2.03	0.40
1:AA:938:U:H2'	1:AA:939:A:H8	1.86	0.40
3:AC:65:ARG:NH1	29:Ak:91:TYR:CE2	2.90	0.40
4:AE:282:ILE:HG21	4:AE:353:LEU:HD13	2.03	0.40
6:AG:121:LYS:NZ	6:AG:210:LEU:HD12	2.37	0.40
8:AJ:81:LYS:HG2	8:AJ:140:TYR:CE1	2.57	0.40
9:AK:113:SER:HB3	9:AK:116:THR:OG1	2.21	0.40
15:AR:75:TYR:CE1	15:AR:114:ARG:HD3	2.56	0.40
17:AV:2:Y5P:H4A	17:AV:3:Y5P:H4	2.04	0.40
17:AV:13:Y5P:H6	17:AV:13:Y5P:OP2	2.22	0.40
17:AY:8:Y5P:H4	17:AY:14:Y5P:H5	2.03	0.40
19:Aa:203:ILE:HB	21:Ac:144:GLU:HB2	2.02	0.40
21:Ac:30:MET:HB3	21:Ac:64:ILE:HG12	2.04	0.40
22:Ad:102:HIS:CD2	22:Ad:106:MET:HE3	2.56	0.40
22:Ad:112:GLU:OE2	22:Ad:115:ARG:NH1	2.55	0.40
23:Ae:234:UNK:O	23:Ae:234:UNK:HG2	2.18	0.40
25:Ag:209:TRP:HB3	25:Ag:231:ARG:NH1	2.36	0.40
28:Aj:95:TRP:HZ3	28:Aj:118:LEU:HD22	1.86	0.40
37:B1:148:THR:HG23	37:B1:152:ASP:HB3	2.03	0.40
37:B1:157:PHE:HE2	66:Ba:48:ARG:NH1	2.19	0.40
38:B2:112:ASN:ND2	64:BX:26:ILE:HB	2.36	0.40
44:B8:113:ARG:HG3	44:B8:114:PHE:CE1	2.57	0.40
46:BA:376:G:N1	46:BA:377:U:C2	2.90	0.40
46:BA:774:C:HO2'	46:BA:775:A:P	2.44	0.40
46:BA:857:A:OP2	48:BD:66:TRP:HZ2	2.05	0.40
46:BA:876:G:C6	46:BA:877:C:C4	3.10	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:BA:1400:C:H4'	49:BE:236:THR:OG1	2.20	0.40
48:BD:185:LEU:HD22	48:BD:217:LEU:HD22	2.04	0.40
49:BE:201:GLY:O	49:BE:202:GLN:HB2	2.20	0.40
52:BJ:67:PRO:HA	52:BJ:68:PRO:HD3	1.89	0.40
54:BN:40:GLN:HA	54:BN:121:MET:HE1	2.03	0.40
54:BN:145:LEU:HA	54:BN:146:PRO:HD3	1.91	0.40
60:BT:268:ASP:O	60:BT:270:MET:N	2.54	0.40
63:BW:51:LYS:HE2	63:BW:51:LYS:HB3	1.83	0.40
64:BX:54:ARG:NH2	86:Bw:308:GLN:O	2.54	0.40
67:Bb:83:GLY:HA3	67:Bb:84:PRO:HD2	1.99	0.40
78:Bm:94:ASP:HB2	78:Bm:97:LEU:HD12	2.03	0.40
88:Bz:412:UNK:HG2	88:Bz:413:UNK:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	218/220 (99%)	212 (97%)	6 (3%)	0	100	100
3	AC	130/132 (98%)	122 (94%)	8 (6%)	0	100	100
4	AE	324/328 (99%)	305 (94%)	18 (6%)	1 (0%)	36	67
5	AF	121/124 (98%)	116 (96%)	5 (4%)	0	100	100
6	AG	206/208 (99%)	203 (98%)	3 (2%)	0	100	100
7	AI	291/311 (94%)	283 (97%)	8 (3%)	0	100	100
8	AJ	127/201 (63%)	119 (94%)	6 (5%)	2 (2%)	7	35
9	AK	134/136 (98%)	128 (96%)	6 (4%)	0	100	100
10	AL	107/109 (98%)	101 (94%)	6 (6%)	0	100	100
11	AN	99/128 (77%)	98 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	AO	173/239 (72%)	166 (96%)	7 (4%)	0	100	100
13	AP	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
14	AQ	107/109 (98%)	102 (95%)	5 (5%)	0	100	100
15	AR	95/97 (98%)	91 (96%)	4 (4%)	0	100	100
16	AU	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
19	Aa	243/356 (68%)	238 (98%)	4 (2%)	1 (0%)	30	62
20	Ab	133/190 (70%)	127 (96%)	6 (4%)	0	100	100
21	Ac	167/169 (99%)	157 (94%)	9 (5%)	1 (1%)	21	54
22	Ad	175/177 (99%)	172 (98%)	3 (2%)	0	100	100
24	Af	97/188 (52%)	90 (93%)	7 (7%)	0	100	100
25	Ag	327/397 (82%)	317 (97%)	10 (3%)	0	100	100
26	Ah	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
27	Ai	97/99 (98%)	90 (93%)	7 (7%)	0	100	100
28	Aj	204/218 (94%)	194 (95%)	10 (5%)	0	100	100
29	Ak	273/275 (99%)	265 (97%)	7 (3%)	1 (0%)	30	62
30	Am	114/116 (98%)	108 (95%)	6 (5%)	0	100	100
31	An	70/72 (97%)	67 (96%)	3 (4%)	0	100	100
32	Ao	87/530 (16%)	83 (95%)	4 (5%)	0	100	100
33	Ap	186/188 (99%)	175 (94%)	11 (6%)	0	100	100
36	B0	112/148 (76%)	109 (97%)	3 (3%)	0	100	100
37	B1	242/256 (94%)	237 (98%)	5 (2%)	0	100	100
38	B2	176/252 (70%)	167 (95%)	9 (5%)	0	100	100
39	B3	116/161 (72%)	112 (97%)	4 (3%)	0	100	100
40	B4	43/126 (34%)	40 (93%)	3 (7%)	0	100	100
41	B5	108/188 (57%)	107 (99%)	1 (1%)	0	100	100
42	B6	46/65 (71%)	45 (98%)	1 (2%)	0	100	100
43	B7	44/95 (46%)	44 (100%)	0	0	100	100
44	B8	93/188 (50%)	90 (97%)	3 (3%)	0	100	100
45	B9	36/100 (36%)	36 (100%)	0	0	100	100
48	BD	238/306 (78%)	228 (96%)	10 (4%)	0	100	100
49	BE	305/348 (88%)	278 (91%)	24 (8%)	3 (1%)	12	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	BF	248/294 (84%)	232 (94%)	16 (6%)	0	100	100
51	BI	96/268 (36%)	91 (95%)	5 (5%)	0	100	100
52	BJ	166/262 (63%)	158 (95%)	8 (5%)	0	100	100
53	BK	140/192 (73%)	134 (96%)	6 (4%)	0	100	100
54	BN	175/178 (98%)	170 (97%)	5 (3%)	0	100	100
55	BO	113/145 (78%)	108 (96%)	5 (4%)	0	100	100
56	BP	286/296 (97%)	273 (96%)	13 (4%)	0	100	100
57	BQ	219/251 (87%)	218 (100%)	1 (0%)	0	100	100
58	BR	151/169 (89%)	145 (96%)	6 (4%)	0	100	100
59	BS	141/180 (78%)	128 (91%)	12 (8%)	1 (1%)	18	51
60	BT	223/292 (76%)	216 (97%)	7 (3%)	0	100	100
61	BU	138/149 (93%)	132 (96%)	6 (4%)	0	100	100
62	BV	153/209 (73%)	146 (95%)	7 (5%)	0	100	100
63	BW	164/210 (78%)	159 (97%)	5 (3%)	0	100	100
64	BX	130/150 (87%)	126 (97%)	4 (3%)	0	100	100
65	BY	202/216 (94%)	190 (94%)	12 (6%)	0	100	100
66	Ba	391/423 (92%)	374 (96%)	17 (4%)	0	100	100
67	Bb	352/380 (93%)	330 (94%)	21 (6%)	1 (0%)	36	67
68	Bc	293/334 (88%)	281 (96%)	12 (4%)	0	100	100
69	Bd	97/206 (47%)	92 (95%)	5 (5%)	0	100	100
70	Be	119/135 (88%)	115 (97%)	4 (3%)	0	100	100
71	Bf	82/142 (58%)	81 (99%)	1 (1%)	0	100	100
72	Bg	146/159 (92%)	138 (94%)	8 (6%)	0	100	100
73	Bh	287/332 (86%)	269 (94%)	18 (6%)	0	100	100
74	Bi	240/312 (77%)	227 (95%)	12 (5%)	1 (0%)	30	62
75	Bj	211/279 (76%)	198 (94%)	12 (6%)	1 (0%)	24	57
76	Bk	132/212 (62%)	125 (95%)	7 (5%)	0	100	100
77	Bl	131/166 (79%)	130 (99%)	1 (1%)	0	100	100
78	Bm	107/159 (67%)	102 (95%)	5 (5%)	0	100	100
79	Bn	95/128 (74%)	91 (96%)	4 (4%)	0	100	100
80	Bo	92/124 (74%)	88 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
81	Bp	95/112 (85%)	90 (95%)	5 (5%)	0	100	100
82	Bq	35/138 (25%)	34 (97%)	1 (3%)	0	100	100
83	Bt	92/102 (90%)	89 (97%)	3 (3%)	0	100	100
84	Bu	137/205 (67%)	129 (94%)	8 (6%)	0	100	100
85	Bv	118/222 (53%)	116 (98%)	2 (2%)	0	100	100
86	Bw	385/433 (89%)	359 (93%)	25 (6%)	1 (0%)	36	67
87	Bx	160/196 (82%)	154 (96%)	5 (3%)	1 (1%)	21	54
All	All	12706/16216 (78%)	12149 (96%)	542 (4%)	15 (0%)	49	79

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
49	BE	264	ILE
86	Bw	159	VAL
87	Bx	93	ILE
8	AJ	179	GLN
8	AJ	185	ARG
49	BE	202	GLN
19	Aa	281	ASP
49	BE	317	PRO
74	Bi	174	TRP
29	Ak	213	ARG
75	Bj	84	TYR
67	Bb	330	VAL
4	AE	154	VAL
21	Ac	105	ILE
59	BS	45	ALA

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	187/187 (100%)	165 (88%)	22 (12%)	5	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AC	115/115 (100%)	96 (84%)	19 (16%)	2	14
4	AE	273/273 (100%)	237 (87%)	36 (13%)	4	19
5	AF	108/109 (99%)	95 (88%)	13 (12%)	5	21
6	AG	181/181 (100%)	165 (91%)	16 (9%)	9	33
7	AI	250/250 (100%)	233 (93%)	17 (7%)	14	40
8	AJ	119/181 (66%)	106 (89%)	13 (11%)	6	25
9	AK	102/102 (100%)	86 (84%)	16 (16%)	2	15
10	AL	92/92 (100%)	80 (87%)	12 (13%)	4	20
11	AN	92/114 (81%)	79 (86%)	13 (14%)	3	18
12	AO	159/205 (78%)	147 (92%)	12 (8%)	12	38
13	AP	97/97 (100%)	91 (94%)	6 (6%)	16	42
14	AQ	94/94 (100%)	84 (89%)	10 (11%)	6	26
15	AR	89/89 (100%)	82 (92%)	7 (8%)	11	36
16	AU	77/77 (100%)	67 (87%)	10 (13%)	4	20
19	Aa	222/272 (82%)	207 (93%)	15 (7%)	14	40
20	Ab	113/162 (70%)	105 (93%)	8 (7%)	13	39
21	Ac	152/152 (100%)	138 (91%)	14 (9%)	8	31
22	Ad	149/149 (100%)	141 (95%)	8 (5%)	20	45
24	Af	86/160 (54%)	79 (92%)	7 (8%)	11	35
25	Ag	290/334 (87%)	263 (91%)	27 (9%)	8	30
26	Ah	95/95 (100%)	93 (98%)	2 (2%)	47	64
27	Ai	86/86 (100%)	77 (90%)	9 (10%)	6	26
28	Aj	182/184 (99%)	172 (94%)	10 (6%)	19	45
29	Ak	249/249 (100%)	224 (90%)	25 (10%)	7	28
30	Am	100/100 (100%)	91 (91%)	9 (9%)	9	32
31	An	66/66 (100%)	57 (86%)	9 (14%)	3	18
32	Ao	79/118 (67%)	73 (92%)	6 (8%)	12	37
33	Ap	168/168 (100%)	152 (90%)	16 (10%)	8	30
36	B0	92/115 (80%)	76 (83%)	16 (17%)	2	12
37	B1	219/229 (96%)	194 (89%)	25 (11%)	5	23
38	B2	164/228 (72%)	143 (87%)	21 (13%)	4	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
39	B3	110/147 (75%)	96 (87%)	14 (13%)	4 21
40	B4	42/114 (37%)	39 (93%)	3 (7%)	13 39
41	B5	99/163 (61%)	91 (92%)	8 (8%)	11 35
42	B6	45/60 (75%)	36 (80%)	9 (20%)	1 8
43	B7	41/78 (53%)	35 (85%)	6 (15%)	3 17
44	B8	87/162 (54%)	76 (87%)	11 (13%)	4 21
45	B9	36/77 (47%)	32 (89%)	4 (11%)	6 24
48	BD	193/248 (78%)	157 (81%)	36 (19%)	1 10
49	BE	263/290 (91%)	238 (90%)	25 (10%)	8 30
50	BF	217/251 (86%)	185 (85%)	32 (15%)	3 17
51	BI	88/228 (39%)	83 (94%)	5 (6%)	18 44
52	BJ	154/230 (67%)	140 (91%)	14 (9%)	9 32
53	BK	115/151 (76%)	109 (95%)	6 (5%)	21 46
54	BN	156/157 (99%)	134 (86%)	22 (14%)	3 18
55	BO	99/123 (80%)	87 (88%)	12 (12%)	5 21
56	BP	245/249 (98%)	204 (83%)	41 (17%)	2 13
57	BQ	189/210 (90%)	167 (88%)	22 (12%)	5 22
58	BR	132/143 (92%)	112 (85%)	20 (15%)	3 16
59	BS	123/153 (80%)	109 (89%)	14 (11%)	5 23
60	BT	206/243 (85%)	178 (86%)	28 (14%)	3 18
61	BU	118/127 (93%)	102 (86%)	16 (14%)	3 18
62	BV	136/178 (76%)	113 (83%)	23 (17%)	2 13
63	BW	144/180 (80%)	121 (84%)	23 (16%)	2 14
64	BX	119/134 (89%)	99 (83%)	20 (17%)	2 13
65	BY	183/192 (95%)	157 (86%)	26 (14%)	3 17
66	Ba	348/365 (95%)	302 (87%)	46 (13%)	4 19
67	Bb	310/328 (94%)	277 (89%)	33 (11%)	6 26
68	Bc	271/299 (91%)	248 (92%)	23 (8%)	10 33
69	Bd	92/181 (51%)	84 (91%)	8 (9%)	9 33
70	Be	100/108 (93%)	87 (87%)	13 (13%)	4 20
71	Bf	80/110 (73%)	67 (84%)	13 (16%)	2 14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
72	Bg	128/136 (94%)	108 (84%)	20 (16%)	2 15
73	Bh	251/284 (88%)	223 (89%)	28 (11%)	6 24
74	Bi	218/281 (78%)	198 (91%)	20 (9%)	8 31
75	Bj	190/242 (78%)	174 (92%)	16 (8%)	10 34
76	Bk	119/181 (66%)	109 (92%)	10 (8%)	10 34
77	Bl	122/147 (83%)	100 (82%)	22 (18%)	2 12
78	Bm	103/145 (71%)	96 (93%)	7 (7%)	14 40
79	Bn	88/113 (78%)	74 (84%)	14 (16%)	2 14
80	Bo	74/97 (76%)	62 (84%)	12 (16%)	2 14
81	Bp	79/88 (90%)	73 (92%)	6 (8%)	12 37
82	Bq	36/114 (32%)	35 (97%)	1 (3%)	38 58
83	Bt	75/82 (92%)	60 (80%)	15 (20%)	1 8
84	Bu	126/169 (75%)	118 (94%)	8 (6%)	16 42
85	Bv	102/173 (59%)	97 (95%)	5 (5%)	22 47
86	Bw	340/373 (91%)	290 (85%)	50 (15%)	3 17
87	Bx	149/173 (86%)	130 (87%)	19 (13%)	4 21
All	All	11288/13510 (84%)	10010 (89%)	1278 (11%)	8 23

All (1278) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AB	57	LEU
2	AB	68	HIS
2	AB	79	SER
2	AB	80	VAL
2	AB	115	ILE
2	AB	133	HIS
2	AB	144	VAL
2	AB	147	HIS
2	AB	149	GLN
2	AB	153	LEU
2	AB	159	ARG
2	AB	168	ARG
2	AB	176	THR
2	AB	177	ASN
2	AB	180	LEU

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Mol	Chain	Res	Type
2	AB	181	LEU
2	AB	195	LEU
2	AB	197	THR
2	AB	206	VAL
2	AB	235	VAL
2	AB	247	LEU
2	AB	253	GLN
3	AC	38	ARG
3	AC	41	ARG
3	AC	44	VAL
3	AC	54	GLU
3	AC	71	LEU
3	AC	77	ASP
3	AC	89	ASP
3	AC	110	LEU
3	AC	112	ARG
3	AC	115	ASN
3	AC	116	GLN
3	AC	117	LEU
3	AC	125	ARG
3	AC	127	LEU
3	AC	132	PHE
3	AC	142	LEU
3	AC	152	HIS
3	AC	163	VAL
3	AC	167	ILE
4	AE	91	THR
4	AE	96	ASP
4	AE	105	GLU
4	AE	131	ILE
4	AE	132	ILE
4	AE	156	THR
4	AE	165	GLN
4	AE	187	VAL
4	AE	215	TYR
4	AE	220	THR
4	AE	228	VAL
4	AE	234	LYS
4	AE	239	ARG
4	AE	242	ARG
4	AE	243	VAL
4	AE	245	VAL

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Mol	Chain	Res	Type
4	AE	266	ASP
4	AE	273	ASN
4	AE	274	ARG
4	AE	276	VAL
4	AE	288	HIS
4	AE	289	THR
4	AE	293	ASP
4	AE	296	LEU
4	AE	300	ARG
4	AE	303	ILE
4	AE	305	MET
4	AE	314	LEU
4	AE	323	ILE
4	AE	336	VAL
4	AE	340	VAL
4	AE	341	ASN
4	AE	370	VAL
4	AE	372	GLU
4	AE	419	ARG
4	AE	420	SER
5	AF	9	ILE
5	AF	17	GLU
5	AF	39	LEU
5	AF	45	ARG
5	AF	65	LEU
5	AF	74	THR
5	AF	86	ILE
5	AF	89	ILE
5	AF	94	VAL
5	AF	105	CYS
5	AF	111	VAL
5	AF	120	THR
5	AF	123	ARG
6	AG	46	ILE
6	AG	47	ASP
6	AG	57	GLU
6	AG	85	VAL
6	AG	98	MET
6	AG	99	MET
6	AG	104	LYS
6	AG	109	SER
6	AG	156	ILE

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Mol	Chain	Res	Type
6	AG	159	VAL
6	AG	197	ARG
6	AG	200	LEU
6	AG	203	GLU
6	AG	205	LEU
6	AG	219	VAL
6	AG	220	ILE
7	AI	70	THR
7	AI	71	VAL
7	AI	99	PHE
7	AI	100	THR
7	AI	202	ILE
7	AI	206	LEU
7	AI	217	GLN
7	AI	229	LEU
7	AI	234	CYS
7	AI	237	THR
7	AI	285	VAL
7	AI	294	ILE
7	AI	308	THR
7	AI	310	ASP
7	AI	314	LEU
7	AI	338	ARG
7	AI	357	VAL
8	AJ	72	LEU
8	AJ	80	VAL
8	AJ	84	ASP
8	AJ	92	GLU
8	AJ	121	LEU
8	AJ	123	SER
8	AJ	126	ILE
8	AJ	136	MET
8	AJ	143	LEU
8	AJ	145	LEU
8	AJ	148	LEU
8	AJ	149	THR
8	AJ	166	GLU
9	AK	65	TYR
9	AK	87	ILE
9	AK	98	GLN
9	AK	107	GLN
9	AK	128	ILE

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Mol	Chain	Res	Type
9	AK	149	VAL
9	AK	151	VAL
9	AK	152	VAL
9	AK	153	VAL
9	AK	160	ARG
9	AK	161	LEU
9	AK	164	ILE
9	AK	175	ILE
9	AK	178	THR
9	AK	194	ARG
9	AK	195	ARG
10	AL	32	THR
10	AL	39	LEU
10	AL	43	LYS
10	AL	52	THR
10	AL	55	ARG
10	AL	61	VAL
10	AL	64	ARG
10	AL	81	CYS
10	AL	103	GLN
10	AL	110	VAL
10	AL	114	ARG
10	AL	135	VAL
11	AN	35	LEU
11	AN	57	LEU
11	AN	58	ARG
11	AN	62	ILE
11	AN	75	ILE
11	AN	81	ASP
11	AN	93	MET
11	AN	101	LYS
11	AN	102	ARG
11	AN	109	ILE
11	AN	120	LEU
11	AN	123	VAL
11	AN	125	ARG
12	AO	72	MET
12	AO	73	LEU
12	AO	80	VAL
12	AO	130	ILE
12	AO	158	LEU
12	AO	161	ILE

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Mol	Chain	Res	Type
12	AO	181	LYS
12	AO	188	ILE
12	AO	198	ARG
12	AO	210	LEU
12	AO	214	VAL
12	AO	218	VAL
13	AP	10	ARG
13	AP	35	VAL
13	AP	44	ASP
13	AP	65	LEU
13	AP	97	TYR
13	AP	110	LEU
14	AQ	13	VAL
14	AQ	18	ILE
14	AQ	30	VAL
14	AQ	55	LEU
14	AQ	57	GLN
14	AQ	59	THR
14	AQ	64	VAL
14	AQ	74	THR
14	AQ	90	GLN
14	AQ	96	THR
15	AR	55	MET
15	AR	56	GLU
15	AR	67	ILE
15	AR	69	CYS
15	AR	91	CYS
15	AR	108	ILE
15	AR	117	ILE
16	AU	27	ASN
16	AU	32	MET
16	AU	33	ASP
16	AU	35	LEU
16	AU	47	LYS
16	AU	50	ARG
16	AU	52	ARG
16	AU	66	MET
16	AU	68	MET
16	AU	77	ARG
19	Aa	103	LYS
19	Aa	106	THR
19	Aa	124	ARG

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Mol	Chain	Res	Type
19	Aa	137	ILE
19	Aa	146	ILE
19	Aa	160	ILE
19	Aa	175	GLU
19	Aa	181	ARG
19	Aa	204	LEU
19	Aa	205	THR
19	Aa	226	VAL
19	Aa	259	ASP
19	Aa	262	ARG
19	Aa	272	TRP
19	Aa	306	LEU
20	Ab	6	LEU
20	Ab	12	ILE
20	Ab	30	LEU
20	Ab	62	ASP
20	Ab	67	GLU
20	Ab	95	THR
20	Ab	109	LEU
20	Ab	112	THR
21	Ac	3	MET
21	Ac	9	ILE
21	Ac	13	LEU
21	Ac	23	PHE
21	Ac	25	ASP
21	Ac	27	VAL
21	Ac	30	MET
21	Ac	31	THR
21	Ac	52	ILE
21	Ac	84	GLU
21	Ac	106	LEU
21	Ac	141	CYS
21	Ac	142	GLU
21	Ac	152	LEU
22	Ad	55	VAL
22	Ad	56	LEU
22	Ad	89	VAL
22	Ad	115	ARG
22	Ad	166	THR
22	Ad	191	ILE
22	Ad	197	VAL
22	Ad	198	VAL

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Mol	Chain	Res	Type
24	Af	85	LEU
24	Af	113	LEU
24	Af	130	VAL
24	Af	145	LEU
24	Af	155	LEU
24	Af	162	THR
24	Af	169	VAL
25	Ag	74	LEU
25	Ag	107	LEU
25	Ag	111	LEU
25	Ag	134	THR
25	Ag	135	LEU
25	Ag	138	CYS
25	Ag	139	HIS
25	Ag	141	LEU
25	Ag	150	LEU
25	Ag	152	LEU
25	Ag	178	ASP
25	Ag	181	LEU
25	Ag	215	THR
25	Ag	225	VAL
25	Ag	231	ARG
25	Ag	243	LEU
25	Ag	246	LEU
25	Ag	264	VAL
25	Ag	265	ASN
25	Ag	281	ILE
25	Ag	296	VAL
25	Ag	305	ILE
25	Ag	311	GLN
25	Ag	336	LEU
25	Ag	337	ASP
25	Ag	382	LEU
25	Ag	397	LEU
26	Ah	302	LEU
26	Ah	314	ASP
27	Ai	11	MET
27	Ai	17	ARG
27	Ai	18	LEU
27	Ai	26	THR
27	Ai	27	ASP
27	Ai	31	MET

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Mol	Chain	Res	Type
27	Ai	62	MET
27	Ai	67	PHE
27	Ai	79	ARG
28	Aj	21	LEU
28	Aj	40	THR
28	Aj	52	MET
28	Aj	65	LEU
28	Aj	80	VAL
28	Aj	133	GLN
28	Aj	164	VAL
28	Aj	170	LEU
28	Aj	184	THR
28	Aj	186	THR
29	Ak	60	GLU
29	Ak	71	VAL
29	Ak	72	TYR
29	Ak	74	VAL
29	Ak	79	LYS
29	Ak	85	LEU
29	Ak	87	VAL
29	Ak	93	VAL
29	Ak	102	GLU
29	Ak	125	CYS
29	Ak	134	GLU
29	Ak	145	CYS
29	Ak	152	GLU
29	Ak	157	ASP
29	Ak	159	VAL
29	Ak	160	SER
29	Ak	165	ILE
29	Ak	213	ARG
29	Ak	216	LEU
29	Ak	234	GLU
29	Ak	264	ILE
29	Ak	288	THR
29	Ak	298	VAL
29	Ak	309	ASN
29	Ak	317	SER
30	Am	6	LEU
30	Am	13	LEU
30	Am	18	ARG
30	Am	29	LEU

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Mol	Chain	Res	Type
30	Am	33	VAL
30	Am	44	THR
30	Am	46	ILE
30	Am	48	GLU
30	Am	64	GLU
31	An	131	LEU
31	An	132	LYS
31	An	133	ILE
31	An	142	LYS
31	An	144	ARG
31	An	145	LYS
31	An	147	VAL
31	An	191	THR
31	An	194	ILE
32	Ao	68	VAL
32	Ao	96	ILE
32	Ao	107	LEU
32	Ao	126	LYS
32	Ao	132	ILE
32	Ao	141	MET
33	Ap	53	ASP
33	Ap	80	ASN
33	Ap	88	GLN
33	Ap	95	ILE
33	Ap	103	ASN
33	Ap	108	CYS
33	Ap	113	LEU
33	Ap	134	ILE
33	Ap	167	ILE
33	Ap	173	ARG
33	Ap	175	LEU
33	Ap	177	PHE
33	Ap	193	LEU
33	Ap	199	TRP
33	Ap	202	TRP
33	Ap	215	ARG
36	B0	40	LYS
36	B0	49	LYS
36	B0	50	ARG
36	B0	53	ILE
36	B0	61	VAL
36	B0	65	ASN

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Mol	Chain	Res	Type
36	B0	66	ILE
36	B0	85	LYS
36	B0	94	GLU
36	B0	122	GLN
36	B0	125	VAL
36	B0	126	LEU
36	B0	131	VAL
36	B0	132	HIS
36	B0	133	VAL
36	B0	147	MET
37	B1	6	VAL
37	B1	32	LEU
37	B1	46	HIS
37	B1	59	ARG
37	B1	61	ARG
37	B1	69	VAL
37	B1	74	GLU
37	B1	93	ASN
37	B1	100	ARG
37	B1	104	VAL
37	B1	116	SER
37	B1	126	THR
37	B1	128	THR
37	B1	155	SER
37	B1	169	LEU
37	B1	172	GLN
37	B1	177	HIS
37	B1	179	ASP
37	B1	190	ARG
37	B1	196	ILE
37	B1	206	LEU
37	B1	216	ARG
37	B1	220	GLU
37	B1	224	ILE
37	B1	231	VAL
38	B2	75	ASN
38	B2	79	GLU
38	B2	89	CYS
38	B2	96	SER
38	B2	132	GLU
38	B2	140	SER
38	B2	141	MET

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Mol	Chain	Res	Type
38	B2	149	GLN
38	B2	150	GLU
38	B2	153	ASP
38	B2	158	LEU
38	B2	160	THR
38	B2	171	ARG
38	B2	174	ILE
38	B2	177	ARG
38	B2	197	ASN
38	B2	204	MET
38	B2	209	ARG
38	B2	228	LEU
38	B2	230	ARG
38	B2	238	GLU
39	B3	41	ILE
39	B3	72	ILE
39	B3	75	THR
39	B3	76	LYS
39	B3	86	ILE
39	B3	99	VAL
39	B3	106	VAL
39	B3	109	LYS
39	B3	118	ARG
39	B3	119	ILE
39	B3	142	ASN
39	B3	144	GLU
39	B3	147	VAL
39	B3	150	LEU
40	B4	42	THR
40	B4	49	TYR
40	B4	57	LEU
41	B5	85	ARG
41	B5	87	ILE
41	B5	103	VAL
41	B5	109	VAL
41	B5	136	GLU
41	B5	153	THR
41	B5	170	GLN
41	B5	186	THR
42	B6	18	VAL
42	B6	20	MET
42	B6	26	THR

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Mol	Chain	Res	Type
42	B6	38	ARG
42	B6	42	THR
42	B6	50	VAL
42	B6	54	VAL
42	B6	55	LEU
42	B6	57	VAL
43	B7	52	ARG
43	B7	61	ILE
43	B7	63	ARG
43	B7	71	ARG
43	B7	79	VAL
43	B7	93	LEU
44	B8	100	ARG
44	B8	106	THR
44	B8	111	ILE
44	B8	116	ARG
44	B8	142	ARG
44	B8	148	VAL
44	B8	163	THR
44	B8	168	ARG
44	B8	174	ASP
44	B8	182	ASP
44	B8	186	LEU
45	B9	63	PHE
45	B9	65	THR
45	B9	70	LYS
45	B9	75	ASP
48	BD	62	THR
48	BD	64	VAL
48	BD	69	ARG
48	BD	70	THR
48	BD	74	VAL
48	BD	82	SER
48	BD	92	GLN
48	BD	111	ARG
48	BD	117	GLU
48	BD	140	ILE
48	BD	148	ARG
48	BD	150	ARG
48	BD	152	ILE
48	BD	153	ILE
48	BD	155	THR

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Mol	Chain	Res	Type
48	BD	167	SER
48	BD	175	VAL
48	BD	178	ARG
48	BD	181	ASP
48	BD	190	VAL
48	BD	213	THR
48	BD	224	THR
48	BD	227	ILE
48	BD	236	GLN
48	BD	239	GLU
48	BD	240	THR
48	BD	245	VAL
48	BD	256	ARG
48	BD	263	ARG
48	BD	265	ARG
48	BD	273	SER
48	BD	277	GLN
48	BD	287	ILE
48	BD	288	ARG
48	BD	290	LEU
48	BD	295	SER
49	BE	46	VAL
49	BE	80	LEU
49	BE	96	ARG
49	BE	109	LEU
49	BE	113	ASP
49	BE	130	LEU
49	BE	146	THR
49	BE	168	LEU
49	BE	181	VAL
49	BE	211	ILE
49	BE	218	VAL
49	BE	227	GLN
49	BE	236	THR
49	BE	237	HIS
49	BE	239	ARG
49	BE	251	VAL
49	BE	273	VAL
49	BE	289	VAL
49	BE	296	LEU
49	BE	304	LEU
49	BE	311	CYS

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Mol	Chain	Res	Type
49	BE	313	ASN
49	BE	318	THR
49	BE	335	GLU
49	BE	345	ILE
50	BF	47	VAL
50	BF	59	ARG
50	BF	62	VAL
50	BF	76	ARG
50	BF	77	VAL
50	BF	79	LEU
50	BF	92	ARG
50	BF	95	ILE
50	BF	101	ILE
50	BF	106	PHE
50	BF	109	ILE
50	BF	110	SER
50	BF	111	TYR
50	BF	114	THR
50	BF	120	VAL
50	BF	129	VAL
50	BF	147	ARG
50	BF	165	LEU
50	BF	167	MET
50	BF	172	GLN
50	BF	190	VAL
50	BF	195	LEU
50	BF	203	LEU
50	BF	215	SER
50	BF	216	VAL
50	BF	234	THR
50	BF	239	THR
50	BF	246	VAL
50	BF	269	LEU
50	BF	277	ASN
50	BF	281	THR
50	BF	292	ASP
51	BI	56	VAL
51	BI	76	ARG
51	BI	82	LEU
51	BI	108	ARG
51	BI	130	VAL
52	BJ	34	THR

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Mol	Chain	Res	Type
52	BJ	60	ILE
52	BJ	63	ARG
52	BJ	65	LEU
52	BJ	73	GLN
52	BJ	76	THR
52	BJ	89	VAL
52	BJ	93	ASN
52	BJ	102	VAL
52	BJ	116	LEU
52	BJ	121	ILE
52	BJ	130	VAL
52	BJ	150	HIS
52	BJ	152	LEU
53	BK	57	THR
53	BK	64	ILE
53	BK	113	THR
53	BK	127	ASP
53	BK	135	VAL
53	BK	137	LEU
54	BN	10	GLN
54	BN	13	THR
54	BN	24	LYS
54	BN	39	LEU
54	BN	49	GLN
54	BN	57	VAL
54	BN	60	MET
54	BN	67	PHE
54	BN	74	GLN
54	BN	78	SER
54	BN	81	THR
54	BN	104	VAL
54	BN	111	MET
54	BN	118	ARG
54	BN	122	MET
54	BN	123	GLN
54	BN	130	ASP
54	BN	140	ASN
54	BN	143	GLU
54	BN	153	ARG
54	BN	154	ARG
54	BN	156	ASP
55	BO	32	ILE

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Mol	Chain	Res	Type
55	BO	48	THR
55	BO	60	VAL
55	BO	73	ILE
55	BO	75	LEU
55	BO	77	ILE
55	BO	91	MET
55	BO	95	ARG
55	BO	102	SER
55	BO	110	ASP
55	BO	121	THR
55	BO	138	LEU
56	BP	11	ARG
56	BP	26	ASN
56	BP	35	LYS
56	BP	37	GLU
56	BP	38	ARG
56	BP	44	ARG
56	BP	49	CYS
56	BP	51	ARG
56	BP	57	ARG
56	BP	58	GLN
56	BP	64	ARG
56	BP	65	LEU
56	BP	71	GLN
56	BP	83	PHE
56	BP	88	SER
56	BP	94	GLN
56	BP	97	SER
56	BP	110	VAL
56	BP	127	VAL
56	BP	130	GLN
56	BP	135	ASP
56	BP	138	VAL
56	BP	139	GLN
56	BP	141	VAL
56	BP	142	GLU
56	BP	146	ASP
56	BP	157	GLN
56	BP	174	VAL
56	BP	175	THR
56	BP	176	THR
56	BP	233	ARG

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Mol	Chain	Res	Type
56	BP	234	LEU
56	BP	238	ARG
56	BP	246	ASP
56	BP	247	ILE
56	BP	250	ASP
56	BP	251	GLU
56	BP	257	SER
56	BP	282	ILE
56	BP	286	THR
56	BP	290	LEU
57	BQ	56	VAL
57	BQ	62	VAL
57	BQ	73	ARG
57	BQ	77	THR
57	BQ	84	GLU
57	BQ	89	ILE
57	BQ	96	TYR
57	BQ	106	ARG
57	BQ	109	ILE
57	BQ	114	ASP
57	BQ	118	MET
57	BQ	131	ILE
57	BQ	144	LYS
57	BQ	147	ILE
57	BQ	171	GLU
57	BQ	204	GLU
57	BQ	209	ASN
57	BQ	214	THR
57	BQ	217	ARG
57	BQ	220	THR
57	BQ	226	ILE
57	BQ	231	SER
58	BR	17	ARG
58	BR	24	SER
58	BR	25	ARG
58	BR	26	ILE
58	BR	28	LEU
58	BR	57	GLU
58	BR	82	GLU
58	BR	84	ASP
58	BR	93	LEU
58	BR	96	ARG

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Mol	Chain	Res	Type
58	BR	98	GLN
58	BR	110	ILE
58	BR	116	GLN
58	BR	118	ARG
58	BR	121	MET
58	BR	134	LEU
58	BR	139	ARG
58	BR	142	ASN
58	BR	143	LEU
58	BR	154	ARG
59	BS	44	VAL
59	BS	52	ASN
59	BS	71	VAL
59	BS	80	ARG
59	BS	103	VAL
59	BS	107	THR
59	BS	112	ILE
59	BS	116	LEU
59	BS	141	ILE
59	BS	145	VAL
59	BS	158	ILE
59	BS	161	LEU
59	BS	171	VAL
59	BS	174	GLU
60	BT	73	THR
60	BT	77	SER
60	BT	79	GLU
60	BT	87	THR
60	BT	90	LEU
60	BT	99	MET
60	BT	105	ILE
60	BT	117	LEU
60	BT	119	VAL
60	BT	130	THR
60	BT	136	ILE
60	BT	138	ILE
60	BT	145	LEU
60	BT	162	ILE
60	BT	165	GLU
60	BT	185	ASN
60	BT	187	LEU
60	BT	196	GLU

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Mol	Chain	Res	Type
60	BT	208	THR
60	BT	219	GLN
60	BT	224	MET
60	BT	246	ASP
60	BT	254	MET
60	BT	260	TRP
60	BT	270	MET
60	BT	272	GLU
60	BT	275	THR
60	BT	282	ILE
61	BU	10	LEU
61	BU	12	SER
61	BU	14	VAL
61	BU	15	THR
61	BU	25	LEU
61	BU	26	LYS
61	BU	32	ARG
61	BU	38	CYS
61	BU	41	LEU
61	BU	46	VAL
61	BU	53	CYS
61	BU	59	LEU
61	BU	64	LEU
61	BU	69	ILE
61	BU	101	VAL
61	BU	102	LEU
62	BV	70	LEU
62	BV	118	ILE
62	BV	120	ILE
62	BV	126	VAL
62	BV	128	CYS
62	BV	133	ARG
62	BV	140	VAL
62	BV	153	LEU
62	BV	156	GLU
62	BV	157	LEU
62	BV	158	VAL
62	BV	159	ARG
62	BV	160	VAL
62	BV	165	ILE
62	BV	176	MET
62	BV	186	ARG

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Mol	Chain	Res	Type
62	BV	190	THR
62	BV	191	VAL
62	BV	195	THR
62	BV	198	ARG
62	BV	199	ILE
62	BV	200	ASN
62	BV	202	ILE
63	BW	67	ARG
63	BW	71	ILE
63	BW	75	ARG
63	BW	77	GLN
63	BW	80	TYR
63	BW	81	SER
63	BW	105	GLU
63	BW	108	ASP
63	BW	118	VAL
63	BW	119	LEU
63	BW	131	ASN
63	BW	135	ARG
63	BW	136	SER
63	BW	145	SER
63	BW	149	GLN
63	BW	152	LYS
63	BW	161	ARG
63	BW	164	ILE
63	BW	170	CYS
63	BW	191	VAL
63	BW	199	GLN
63	BW	206	ILE
63	BW	207	THR
64	BX	5	VAL
64	BX	14	ASN
64	BX	17	LEU
64	BX	18	ARG
64	BX	26	ILE
64	BX	35	GLN
64	BX	39	THR
64	BX	40	VAL
64	BX	48	MET
64	BX	49	THR
64	BX	57	LEU
64	BX	71	ARG

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Mol	Chain	Res	Type
64	BX	77	ASN
64	BX	79	ARG
64	BX	85	ILE
64	BX	104	THR
64	BX	109	ASP
64	BX	141	ARG
64	BX	148	PHE
64	BX	150	LEU
65	BY	29	LEU
65	BY	40	ARG
65	BY	44	VAL
65	BY	66	GLU
65	BY	69	ASP
65	BY	78	GLN
65	BY	79	VAL
65	BY	86	VAL
65	BY	96	ARG
65	BY	105	ARG
65	BY	131	THR
65	BY	137	PHE
65	BY	138	THR
65	BY	144	VAL
65	BY	145	ARG
65	BY	149	ARG
65	BY	153	ILE
65	BY	163	ASP
65	BY	166	VAL
65	BY	181	ASP
65	BY	186	THR
65	BY	193	THR
65	BY	202	MET
65	BY	208	ARG
65	BY	209	ARG
65	BY	216	TYR
66	Ba	42	GLU
66	Ba	49	VAL
66	Ba	64	MET
66	Ba	67	MET
66	Ba	72	ARG
66	Ba	74	VAL
66	Ba	102	GLN
66	Ba	111	CYS

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Mol	Chain	Res	Type
66	Ba	124	THR
66	Ba	128	LEU
66	Ba	147	ILE
66	Ba	149	ASN
66	Ba	151	ASP
66	Ba	163	LEU
66	Ba	167	THR
66	Ba	169	ASP
66	Ba	175	THR
66	Ba	180	ILE
66	Ba	185	ILE
66	Ba	202	ILE
66	Ba	210	SER
66	Ba	222	VAL
66	Ba	256	PHE
66	Ba	259	ILE
66	Ba	268	CYS
66	Ba	270	VAL
66	Ba	277	THR
66	Ba	280	GLN
66	Ba	307	ASP
66	Ba	316	PHE
66	Ba	334	LYS
66	Ba	335	VAL
66	Ba	336	LEU
66	Ba	337	GLU
66	Ba	342	VAL
66	Ba	347	THR
66	Ba	355	LEU
66	Ba	370	VAL
66	Ba	372	ASN
66	Ba	376	VAL
66	Ba	388	CYS
66	Ba	391	VAL
66	Ba	396	VAL
66	Ba	398	VAL
66	Ba	404	ILE
66	Ba	415	LEU
67	Bb	40	ILE
67	Bb	51	TYR
67	Bb	52	ARG
67	Bb	53	SER

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Mol	Chain	Res	Type
67	Bb	90	ILE
67	Bb	97	VAL
67	Bb	118	GLU
67	Bb	130	ILE
67	Bb	153	GLU
67	Bb	175	VAL
67	Bb	185	MET
67	Bb	209	ASP
67	Bb	210	GLU
67	Bb	222	ASP
67	Bb	240	ILE
67	Bb	245	VAL
67	Bb	258	PHE
67	Bb	261	ARG
67	Bb	279	ILE
67	Bb	281	PHE
67	Bb	284	ASP
67	Bb	288	SER
67	Bb	303	PHE
67	Bb	312	THR
67	Bb	322	ARG
67	Bb	324	ASP
67	Bb	329	ARG
67	Bb	334	LEU
67	Bb	335	LEU
67	Bb	337	MET
67	Bb	356	ARG
67	Bb	376	THR
67	Bb	379	ILE
68	Bc	56	THR
68	Bc	67	VAL
68	Bc	98	ARG
68	Bc	106	ASP
68	Bc	111	ASP
68	Bc	122	ILE
68	Bc	129	ASP
68	Bc	131	ASP
68	Bc	140	TRP
68	Bc	142	SER
68	Bc	143	CYS
68	Bc	157	ASP
68	Bc	177	CYS

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Mol	Chain	Res	Type
68	Bc	190	MET
68	Bc	218	VAL
68	Bc	222	VAL
68	Bc	229	HIS
68	Bc	256	ASP
68	Bc	280	VAL
68	Bc	285	THR
68	Bc	291	ARG
68	Bc	310	ASN
68	Bc	319	MET
69	Bd	89	ILE
69	Bd	104	VAL
69	Bd	118	LEU
69	Bd	123	LEU
69	Bd	136	ILE
69	Bd	139	LEU
69	Bd	150	LEU
69	Bd	162	THR
70	Be	23	SER
70	Be	28	ARG
70	Be	60	VAL
70	Be	62	GLU
70	Be	63	LEU
70	Be	66	PHE
70	Be	68	LEU
70	Be	72	VAL
70	Be	78	GLU
70	Be	106	THR
70	Be	111	HIS
70	Be	118	GLU
70	Be	127	GLN
71	Bf	39	LEU
71	Bf	44	ASN
71	Bf	56	ARG
71	Bf	59	VAL
71	Bf	64	SER
71	Bf	102	HIS
71	Bf	108	MET
71	Bf	109	ILE
71	Bf	122	ARG
71	Bf	126	ARG
71	Bf	131	ARG

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Mol	Chain	Res	Type
71	Bf	134	ARG
71	Bf	135	LYS
72	Bg	6	THR
72	Bg	12	THR
72	Bg	14	VAL
72	Bg	21	ARG
72	Bg	33	LEU
72	Bg	34	SER
72	Bg	65	VAL
72	Bg	68	ARG
72	Bg	70	CYS
72	Bg	89	ILE
72	Bg	93	SER
72	Bg	108	SER
72	Bg	112	VAL
72	Bg	113	ILE
72	Bg	117	LYS
72	Bg	119	PHE
72	Bg	125	SER
72	Bg	126	ILE
72	Bg	127	GLN
72	Bg	148	VAL
73	Bh	33	LYS
73	Bh	42	GLN
73	Bh	45	LEU
73	Bh	51	LEU
73	Bh	53	CYS
73	Bh	78	ARG
73	Bh	82	THR
73	Bh	84	SER
73	Bh	96	CYS
73	Bh	98	ILE
73	Bh	121	ASP
73	Bh	145	PHE
73	Bh	153	VAL
73	Bh	191	LEU
73	Bh	213	LEU
73	Bh	216	ARG
73	Bh	231	MET
73	Bh	233	THR
73	Bh	251	SER
73	Bh	259	ARG

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Mol	Chain	Res	Type
73	Bh	263	SER
73	Bh	267	LEU
73	Bh	288	THR
73	Bh	289	VAL
73	Bh	293	GLU
73	Bh	294	GLU
73	Bh	301	LEU
73	Bh	304	LEU
74	Bi	65	LEU
74	Bi	74	ARG
74	Bi	144	ILE
74	Bi	165	THR
74	Bi	171	ASP
74	Bi	175	ASP
74	Bi	181	VAL
74	Bi	186	VAL
74	Bi	196	GLN
74	Bi	208	ILE
74	Bi	221	THR
74	Bi	230	ARG
74	Bi	237	ASP
74	Bi	238	VAL
74	Bi	242	VAL
74	Bi	244	GLU
74	Bi	246	VAL
74	Bi	258	SER
74	Bi	276	ILE
74	Bi	280	VAL
75	Bj	51	LEU
75	Bj	55	ARG
75	Bj	60	THR
75	Bj	89	LEU
75	Bj	137	LEU
75	Bj	139	GLU
75	Bj	145	ASP
75	Bj	169	ASP
75	Bj	179	GLN
75	Bj	195	LEU
75	Bj	231	VAL
75	Bj	255	VAL
75	Bj	264	LEU
75	Bj	265	LYS

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Mol	Chain	Res	Type
75	Bj	274	ARG
75	Bj	276	LEU
76	Bk	49	ARG
76	Bk	50	SER
76	Bk	81	ASN
76	Bk	92	ASN
76	Bk	100	MET
76	Bk	147	ASP
76	Bk	150	LEU
76	Bk	156	VAL
76	Bk	165	THR
76	Bk	184	LEU
77	Bl	42	VAL
77	Bl	48	VAL
77	Bl	57	ILE
77	Bl	73	GLN
77	Bl	77	ASP
77	Bl	89	SER
77	Bl	94	ILE
77	Bl	100	ILE
77	Bl	101	THR
77	Bl	108	THR
77	Bl	111	ARG
77	Bl	113	VAL
77	Bl	117	ILE
77	Bl	125	GLU
77	Bl	128	LEU
77	Bl	131	LEU
77	Bl	137	VAL
77	Bl	138	THR
77	Bl	141	ASN
77	Bl	143	VAL
77	Bl	155	GLN
77	Bl	163	GLU
78	Bm	52	VAL
78	Bm	56	ILE
78	Bm	67	LEU
78	Bm	121	MET
78	Bm	126	ASP
78	Bm	142	ASP
78	Bm	144	LEU
79	Bn	32	PHE

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Mol	Chain	Res	Type
79	Bn	34	VAL
79	Bn	44	VAL
79	Bn	46	ARG
79	Bn	48	ASN
79	Bn	53	MET
79	Bn	56	VAL
79	Bn	60	ILE
79	Bn	66	PHE
79	Bn	78	ILE
79	Bn	92	ILE
79	Bn	98	VAL
79	Bn	104	ILE
79	Bn	105	ASP
80	Bo	25	SER
80	Bo	26	GLN
80	Bo	31	GLN
80	Bo	40	TYR
80	Bo	43	LEU
80	Bo	44	THR
80	Bo	64	LEU
80	Bo	65	ARG
80	Bo	72	LYS
80	Bo	77	VAL
80	Bo	84	MET
80	Bo	110	LEU
81	Bp	15	GLN
81	Bp	28	GLU
81	Bp	55	VAL
81	Bp	75	ILE
81	Bp	82	THR
81	Bp	84	GLN
82	Bq	121	LEU
83	Bt	9	ARG
83	Bt	10	ASN
83	Bt	16	GLN
83	Bt	18	ILE
83	Bt	25	ARG
83	Bt	27	VAL
83	Bt	35	MET
83	Bt	40	GLU
83	Bt	45	ASN
83	Bt	55	THR

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Mol	Chain	Res	Type
83	Bt	57	GLU
83	Bt	81	ARG
83	Bt	88	LEU
83	Bt	97	VAL
83	Bt	99	ARG
84	Bu	56	ASP
84	Bu	97	LYS
84	Bu	123	LYS
84	Bu	138	CYS
84	Bu	140	ARG
84	Bu	153	LEU
84	Bu	159	GLU
84	Bu	184	ARG
85	Bv	38	ARG
85	Bv	47	THR
85	Bv	52	LEU
85	Bv	59	LYS
85	Bv	74	SER
86	Bw	43	ARG
86	Bw	51	LEU
86	Bw	55	SER
86	Bw	77	ASP
86	Bw	81	ARG
86	Bw	92	VAL
86	Bw	96	GLN
86	Bw	100	LEU
86	Bw	118	LEU
86	Bw	153	ARG
86	Bw	162	ASP
86	Bw	166	ILE
86	Bw	194	LEU
86	Bw	196	CYS
86	Bw	216	ARG
86	Bw	236	ARG
86	Bw	237	ILE
86	Bw	241	LEU
86	Bw	245	VAL
86	Bw	248	ASP
86	Bw	258	MET
86	Bw	263	ASP
86	Bw	267	LEU
86	Bw	270	ARG

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Mol	Chain	Res	Type
86	Bw	271	GLN
86	Bw	274	ASN
86	Bw	278	ILE
86	Bw	282	THR
86	Bw	291	THR
86	Bw	306	LEU
86	Bw	315	GLU
86	Bw	326	LEU
86	Bw	330	THR
86	Bw	335	MET
86	Bw	336	TYR
86	Bw	347	ARG
86	Bw	368	LEU
86	Bw	376	GLN
86	Bw	378	ASP
86	Bw	383	ARG
86	Bw	395	LEU
86	Bw	397	GLU
86	Bw	398	THR
86	Bw	399	ILE
86	Bw	402	ASN
86	Bw	404	VAL
86	Bw	405	LYS
86	Bw	410	ASP
86	Bw	420	LEU
86	Bw	421	ASN
87	Bx	38	VAL
87	Bx	54	THR
87	Bx	73	CYS
87	Bx	89	LEU
87	Bx	92	PHE
87	Bx	93	ILE
87	Bx	100	LEU
87	Bx	111	GLU
87	Bx	115	ILE
87	Bx	123	HIS
87	Bx	128	LEU
87	Bx	130	ASN
87	Bx	148	ASN
87	Bx	149	ARG
87	Bx	152	THR
87	Bx	155	SER

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Mol	Chain	Res	Type
87	Bx	162	ILE
87	Bx	190	ARG
87	Bx	193	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (302) such sidechains are listed below:

Mol	Chain	Res	Type
2	AB	92	HIS
2	AB	129	ASN
2	AB	133	HIS
2	AB	152	HIS
2	AB	215	ASN
3	AC	57	HIS
3	AC	72	HIS
3	AC	75	ASN
3	AC	115	ASN
3	AC	154	HIS
3	AC	156	GLN
4	AE	130	GLN
4	AE	145	ASN
4	AE	155	GLN
4	AE	196	ASN
4	AE	277	HIS
4	AE	288	HIS
4	AE	292	HIS
4	AE	359	HIS
4	AE	369	HIS
5	AF	54	HIS
5	AF	58	HIS
6	AG	146	HIS
6	AG	227	HIS
6	AG	233	ASN
7	AI	87	HIS
7	AI	90	ASN
7	AI	127	HIS
7	AI	148	HIS
7	AI	156	GLN
7	AI	163	HIS
7	AI	313	GLN
7	AI	327	HIS
7	AI	367	GLN
8	AJ	83	HIS

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Mol	Chain	Res	Type
8	AJ	161	GLN
8	AJ	183	HIS
9	AK	71	GLN
9	AK	95	ASN
10	AL	35	GLN
10	AL	44	HIS
10	AL	57	GLN
10	AL	134	HIS
11	AN	60	ASN
11	AN	117	HIS
11	AN	124	GLN
12	AO	145	GLN
12	AO	153	HIS
13	AP	28	ASN
13	AP	69	ASN
14	AQ	9	HIS
14	AQ	23	GLN
14	AQ	56	GLN
14	AQ	57	GLN
15	AR	72	HIS
15	AR	83	GLN
16	AU	3	ASN
16	AU	27	ASN
16	AU	79	ASN
16	AU	85	GLN
19	Aa	75	GLN
19	Aa	107	GLN
19	Aa	222	GLN
19	Aa	228	ASN
19	Aa	247	HIS
19	Aa	287	GLN
21	Ac	33	ASN
21	Ac	51	ASN
21	Ac	56	GLN
21	Ac	59	ASN
21	Ac	63	GLN
21	Ac	69	ASN
21	Ac	95	ASN
21	Ac	101	HIS
21	Ac	125	HIS
21	Ac	146	GLN
22	Ad	31	HIS

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Mol	Chain	Res	Type
22	Ad	65	GLN
22	Ad	102	HIS
22	Ad	109	ASN
22	Ad	117	HIS
22	Ad	159	GLN
22	Ad	161	GLN
24	Af	98	ASN
25	Ag	80	HIS
25	Ag	153	HIS
25	Ag	173	ASN
25	Ag	210	ASN
25	Ag	249	GLN
25	Ag	290	HIS
25	Ag	348	ASN
25	Ag	357	GLN
25	Ag	386	ASN
25	Ag	389	GLN
26	Ah	323	HIS
27	Ai	56	ASN
27	Ai	75	HIS
29	Ak	104	ASN
29	Ak	187	HIS
29	Ak	263	ASN
29	Ak	303	ASN
30	Am	24	ASN
30	Am	31	ASN
30	Am	109	HIS
30	Am	113	ASN
30	Am	116	HIS
31	An	129	ASN
31	An	140	HIS
31	An	178	GLN
32	Ao	122	ASN
32	Ao	129	GLN
33	Ap	66	ASN
33	Ap	130	HIS
33	Ap	136	HIS
33	Ap	147	HIS
36	B0	59	HIS
36	B0	76	HIS
37	B1	27	HIS
37	B1	42	HIS

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Mol	Chain	Res	Type
37	B1	94	ASN
37	B1	172	GLN
38	B2	75	ASN
38	B2	90	GLN
38	B2	197	ASN
39	B3	142	ASN
40	B4	37	ASN
41	B5	83	ASN
41	B5	144	GLN
41	B5	170	GLN
42	B6	45	HIS
43	B7	65	HIS
48	BD	169	HIS
48	BD	196	ASN
49	BE	72	GLN
49	BE	128	HIS
49	BE	156	HIS
49	BE	174	GLN
49	BE	197	HIS
49	BE	202	GLN
49	BE	216	GLN
49	BE	281	ASN
49	BE	292	HIS
50	BF	63	GLN
50	BF	74	GLN
50	BF	83	HIS
50	BF	97	HIS
50	BF	103	GLN
50	BF	105	ASN
50	BF	130	GLN
50	BF	153	HIS
50	BF	172	GLN
50	BF	201	GLN
50	BF	241	ASN
50	BF	249	ASN
50	BF	251	HIS
51	BI	88	HIS
51	BI	136	ASN
52	BJ	41	HIS
52	BJ	93	ASN
52	BJ	119	HIS
53	BK	54	ASN

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Mol	Chain	Res	Type
53	BK	84	GLN
53	BK	103	HIS
54	BN	70	ASN
54	BN	74	GLN
54	BN	80	HIS
54	BN	96	HIS
55	BO	103	ASN
56	BP	53	HIS
56	BP	71	GLN
56	BP	157	GLN
56	BP	170	ASN
56	BP	198	GLN
57	BQ	98	HIS
57	BQ	110	ASN
57	BQ	209	ASN
57	BQ	237	HIS
58	BR	11	HIS
58	BR	27	HIS
58	BR	39	HIS
58	BR	112	ASN
59	BS	52	ASN
59	BS	147	HIS
60	BT	212	ASN
60	BT	218	ASN
60	BT	291	ASN
61	BU	22	GLN
61	BU	77	GLN
61	BU	94	GLN
62	BV	79	HIS
62	BV	88	ASN
62	BV	104	HIS
62	BV	108	HIS
62	BV	109	GLN
62	BV	200	ASN
63	BW	99	GLN
63	BW	123	GLN
63	BW	171	HIS
63	BW	203	ASN
64	BX	14	ASN
64	BX	73	GLN
64	BX	77	ASN
65	BY	35	ASN

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Mol	Chain	Res	Type
65	BY	78	GLN
65	BY	84	ASN
65	BY	117	HIS
66	Ba	108	HIS
66	Ba	150	GLN
66	Ba	156	ASN
66	Ba	195	HIS
66	Ba	207	ASN
66	Ba	221	GLN
66	Ba	223	HIS
66	Ba	266	GLN
66	Ba	269	ASN
66	Ba	289	HIS
66	Ba	324	GLN
66	Ba	358	GLN
67	Bb	224	HIS
67	Bb	266	HIS
67	Bb	275	GLN
67	Bb	320	GLN
67	Bb	354	GLN
68	Bc	81	ASN
68	Bc	229	HIS
68	Bc	230	ASN
68	Bc	243	GLN
68	Bc	252	HIS
68	Bc	282	ASN
68	Bc	294	GLN
68	Bc	305	HIS
68	Bc	310	ASN
69	Bd	143	GLN
70	Be	42	HIS
70	Be	50	GLN
70	Be	132	ASN
71	Bf	44	ASN
71	Bf	62	HIS
71	Bf	121	HIS
72	Bg	17	ASN
72	Bg	127	GLN
72	Bg	131	HIS
72	Bg	135	ASN
73	Bh	42	GLN
73	Bh	73	GLN

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Mol	Chain	Res	Type
73	Bh	94	ASN
73	Bh	118	ASN
73	Bh	177	GLN
73	Bh	222	GLN
73	Bh	260	GLN
73	Bh	310	ASN
74	Bi	119	GLN
74	Bi	193	GLN
74	Bi	196	GLN
75	Bj	87	HIS
75	Bj	150	HIS
75	Bj	198	ASN
75	Bj	251	HIS
75	Bj	252	HIS
76	Bk	54	HIS
76	Bk	92	ASN
76	Bk	94	HIS
76	Bk	158	GLN
76	Bk	175	HIS
76	Bk	177	ASN
76	Bk	189	HIS
77	Bl	141	ASN
78	Bm	96	HIS
78	Bm	136	GLN
79	Bn	69	HIS
79	Bn	122	ASN
80	Bo	63	GLN
81	Bp	15	GLN
81	Bp	72	HIS
82	Bq	125	ASN
82	Bq	129	HIS
83	Bt	30	GLN
83	Bt	34	ASN
83	Bt	45	ASN
83	Bt	78	GLN
83	Bt	85	HIS
83	Bt	91	GLN
84	Bu	103	HIS
84	Bu	122	HIS
84	Bu	124	ASN
84	Bu	145	ASN
84	Bu	183	ASN

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Mol	Chain	Res	Type
86	Bw	71	HIS
86	Bw	101	ASN
86	Bw	104	ASN
86	Bw	107	GLN
86	Bw	146	GLN
86	Bw	185	HIS
86	Bw	228	ASN
86	Bw	271	GLN
86	Bw	292	GLN
86	Bw	321	ASN
86	Bw	385	ASN
86	Bw	421	ASN
87	Bx	164	ASN
87	Bx	170	ASN
87	Bx	184	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	959/962 (99%)	308 (32%)	7 (0%)
17	AV	66/69 (95%)	12 (18%)	0
17	AY	65/69 (94%)	16 (24%)	0
18	AX	12/13 (92%)	4 (33%)	0
46	BA	1508/1570 (96%)	622 (41%)	30 (1%)
47	BB	48/51 (94%)	13 (27%)	0
All	All	2658/2734 (97%)	975 (36%)	37 (1%)

All (975) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	A
1	AA	10	U
1	AA	11	G
1	AA	14	C
1	AA	18	G
1	AA	34	U
1	AA	36	A
1	AA	39	A
1	AA	42	A
1	AA	45	A
1	AA	49	A

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Mol	Chain	Res	Type
1	AA	51	G
1	AA	54	A
1	AA	55	G
1	AA	58	U
1	AA	61	G
1	AA	63	G
1	AA	65	C
1	AA	77	G
1	AA	78	C
1	AA	83	C
1	AA	92	A
1	AA	98	A
1	AA	102	G
1	AA	104	A
1	AA	111	A
1	AA	115	A
1	AA	118	A
1	AA	120	A
1	AA	124	A
1	AA	125	U
1	AA	126	A
1	AA	127	A
1	AA	128	C
1	AA	129	G
1	AA	139	A
1	AA	142	G
1	AA	147	G
1	AA	151	A
1	AA	152	A
1	AA	160	C
1	AA	161	C
1	AA	162	C
1	AA	163	A
1	AA	165	G
1	AA	168	A
1	AA	170	A
1	AA	171	C
1	AA	173	G
1	AA	175	A
1	AA	184	A
1	AA	186	U
1	AA	191	C

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Mol	Chain	Res	Type
1	AA	192	C
1	AA	194	U
1	AA	198	C
1	AA	199	G
1	AA	202	A
1	AA	203	G
1	AA	216	A
1	AA	217	U
1	AA	222	A
1	AA	223	U
1	AA	224	U
1	AA	225	A
1	AA	227	A
1	AA	231	G
1	AA	237	U
1	AA	238	C
1	AA	244	C
1	AA	245	C
1	AA	246	A
1	AA	247	G
1	AA	253	G
1	AA	257	U
1	AA	258	C
1	AA	259	A
1	AA	265	U
1	AA	273	A
1	AA	281	G
1	AA	285	C
1	AA	286	A
1	AA	288	G
1	AA	293	A
1	AA	294	A
1	AA	297	A
1	AA	298	G
1	AA	309	A
1	AA	310	A
1	AA	311	A
1	AA	313	A
1	AA	316	C
1	AA	317	A
1	AA	318	C
1	AA	319	A

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Mol	Chain	Res	Type
1	AA	320	A
1	AA	330	A
1	AA	340	A
1	AA	345	U
1	AA	354	C
1	AA	360	A
1	AA	361	A
1	AA	362	A
1	AA	367	A
1	AA	368	A
1	AA	369	U
1	AA	372	C
1	AA	381	G
1	AA	392	A
1	AA	393	A
1	AA	394	U
1	AA	395	C
1	AA	396	C
1	AA	399	A
1	AA	400	C
1	AA	417	C
1	AA	421	A
1	AA	425	G
1	AA	433	U
1	AA	434	A
1	AA	439	A
1	AA	444	G
1	AA	445	C
1	AA	448	A
1	AA	454	A
1	AA	455	A
1	AA	456	A
1	AA	457	C
1	AA	458	C
1	AA	459	C
1	AA	461	A
1	AA	465	G
1	AA	471	U
1	AA	472	A
1	AA	477	A
1	AA	479	C
1	AA	481	A

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Mol	Chain	Res	Type
1	AA	487	C
1	AA	488	A
1	AA	489	G
1	AA	493	A
1	AA	498	U
1	AA	501	C
1	AA	502	A
1	AA	504	C
1	AA	505	U
1	AA	506	G
1	AA	513	A
1	AA	515	U
1	AA	517	A
1	AA	518	A
1	AA	526	G
1	AA	530	G
1	AA	536	C
1	AA	538	C
1	AA	540	U
1	AA	547	A
1	AA	559	U
1	AA	561	U
1	AA	562	A
1	AA	564	A
1	AA	566	U
1	AA	571	A
1	AA	574	C
1	AA	576	C
1	AA	577	C
1	AA	579	A
1	AA	581	A
1	AA	582	G
1	AA	588	A
1	AA	589	C
1	AA	592	A
1	AA	593	C
1	AA	594	C
1	AA	597	U
1	AA	604	U
1	AA	606	A
1	AA	607	G
1	AA	609	C

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Mol	Chain	Res	Type
1	AA	610	U
1	AA	612	U
1	AA	613	A
1	AA	619	C
1	AA	620	C
1	AA	625	U
1	AA	626	C
1	AA	627	A
1	AA	628	G
1	AA	630	A
1	AA	633	C
1	AA	635	C
1	AA	637	A
1	AA	638	A
1	AA	639	A
1	AA	640	A
1	AA	644	A
1	AA	645	A
1	AA	646	C
1	AA	647	A
1	AA	648	A
1	AA	649	U
1	AA	650	A
1	AA	654	A
1	AA	655	G
1	AA	656	C
1	AA	661	U
1	AA	662	C
1	AA	665	A
1	AA	666	G
1	AA	667	C
1	AA	669	C
1	AA	681	A
1	AA	682	G
1	AA	686	A
1	AA	693	A
1	AA	694	G
1	AA	695	C
1	AA	698	A
1	AA	707	A
1	AA	708	A
1	AA	711	A

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Mol	Chain	Res	Type
1	AA	720	A
1	AA	722	A
1	AA	723	U
1	AA	732	U
1	AA	733	A
1	AA	734	A
1	AA	739	A
1	AA	740	U
1	AA	742	C
1	AA	744	C
1	AA	745	C
1	AA	746	A
1	AA	747	C
1	AA	748	A
1	AA	752	A
1	AA	753	A
1	AA	761	U
1	AA	765	A
1	AA	766	C
1	AA	775	A
1	AA	790	A
1	AA	791	G
1	AA	802	A
1	AA	803	U
1	AA	804	A
1	AA	807	G
1	AA	808	U
1	AA	821	A
1	AA	822	A
1	AA	823	G
1	AA	824	G
1	AA	825	C
1	AA	826	C
1	AA	835	C
1	AA	838	A
1	AA	841	C
1	AA	842	A
1	AA	861	A
1	AA	862	A
1	AA	863	G
1	AA	867	G
1	AA	868	U

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Mol	Chain	Res	Type
1	AA	869	A
1	AA	870	G
1	AA	874	U
1	AA	875	A
1	AA	876	A
1	AA	877	A
1	AA	878	A
1	AA	880	U
1	AA	881	A
1	AA	884	C
1	AA	885	U
1	AA	886	A
1	AA	890	U
1	AA	891	C
1	AA	894	U
1	AA	895	U
1	AA	896	A
1	AA	897	C
1	AA	898	A
1	AA	899	C
1	AA	900	A
1	AA	901	A
1	AA	902	C
1	AA	910	G
1	AA	912	A
1	AA	915	G
1	AA	917	C
1	AA	918	A
1	AA	919	A
1	AA	920	G
1	AA	923	G
1	AA	925	A
1	AA	928	A
1	AA	930	G
1	AA	932	U
1	AA	933	A
1	AA	934	A
1	AA	943	G
1	AA	945	A
1	AA	946	A
1	AA	955	G
1	AA	956	G

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Mol	Chain	Res	Type
1	AA	958	U
1	AA	959	U
1	AA	962	C
17	AV	6	Y5P
17	AV	8	Y5P
17	AV	9	Y5P
17	AV	22	Y5P
17	AV	23	Y5P
17	AV	32	Y5P
17	AV	42	Y5P
17	AV	52	Y5P
17	AV	59	Y5P
17	AV	69	Y5P
17	AV	75	Y5P
17	AV	76	P5P
18	AX	13	Y5P
18	AX	15	Y5P
18	AX	23	Y5P
18	AX	24	Y5P
17	AY	3	Y5P
17	AY	9	Y5P
17	AY	15	Y5P
17	AY	23	Y5P
17	AY	30	Y5P
17	AY	34	P5P
17	AY	42	Y5P
17	AY	43	Y5P
17	AY	52	Y5P
17	AY	53	Y5P
17	AY	57	Y5P
17	AY	67	Y5P
17	AY	68	Y5P
17	AY	73	Y5P
17	AY	74	Y5P
17	AY	75	Y5P
46	BA	4	A
46	BA	5	A
46	BA	7	G
46	BA	11	G
46	BA	16	A
46	BA	27	A
46	BA	30	U

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Mol	Chain	Res	Type
46	BA	31	A
46	BA	32	C
46	BA	36	A
46	BA	37	A
46	BA	39	A
46	BA	40	C
46	BA	41	A
46	BA	42	C
46	BA	43	C
46	BA	44	A
46	BA	45	A
46	BA	46	A
46	BA	48	U
46	BA	49	A
46	BA	54	A
46	BA	56	A
46	BA	57	A
46	BA	58	C
46	BA	59	A
46	BA	60	U
46	BA	61	U
46	BA	63	A
46	BA	66	U
46	BA	67	A
46	BA	68	A
46	BA	69	C
46	BA	70	A
46	BA	71	U
46	BA	72	U
46	BA	82	G
46	BA	83	A
46	BA	84	G
46	BA	96	U
46	BA	97	A
46	BA	98	U
46	BA	99	C
46	BA	100	C
46	BA	101	U
46	BA	102	G
46	BA	104	C
46	BA	105	G
46	BA	108	A

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Mol	Chain	Res	Type
46	BA	109	U
46	BA	110	A
46	BA	112	A
46	BA	113	G
46	BA	115	U
46	BA	116	A
46	BA	117	G
46	BA	119	A
46	BA	128	A
46	BA	129	A
46	BA	131	G
46	BA	133	U
46	BA	136	A
46	BA	138	G
46	BA	139	A
46	BA	140	A
46	BA	148	A
46	BA	152	U
46	BA	156	A
46	BA	157	A
46	BA	158	A
46	BA	159	A
46	BA	160	A
46	BA	161	G
46	BA	162	C
46	BA	163	A
46	BA	164	A
46	BA	167	A
46	BA	168	U
46	BA	169	U
46	BA	171	C
46	BA	178	U
46	BA	179	A
46	BA	187	C
46	BA	189	U
46	BA	191	A
46	BA	203	G
46	BA	204	A
46	BA	206	A
46	BA	207	A
46	BA	209	A
46	BA	217	A

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Mol	Chain	Res	Type
46	BA	218	A
46	BA	219	G
46	BA	220	A
46	BA	222	A
46	BA	223	A
46	BA	224	C
46	BA	225	U
46	BA	227	U
46	BA	228	A
46	BA	229	G
46	BA	230	C
46	BA	236	A
46	BA	237	C
46	BA	238	C
46	BA	242	A
46	BA	253	G
46	BA	258	C
46	BA	262	G
46	BA	270	U
46	BA	271	A
46	BA	272	A
46	BA	274	A
46	BA	275	G
46	BA	276	A
46	BA	277	A
46	BA	293	G
46	BA	294	G
46	BA	295	C
46	BA	302	G
46	BA	305	A
46	BA	308	A
46	BA	310	A
46	BA	311	C
46	BA	321	G
46	BA	322	A
46	BA	323	G
46	BA	328	A
46	BA	329	A
46	BA	330	A
46	BA	331	G
46	BA	335	A
46	BA	336	A

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Mol	Chain	Res	Type
46	BA	337	C
46	BA	338	G
46	BA	339	A
46	BA	344	G
46	BA	347	G
46	BA	348	A
46	BA	351	G
46	BA	356	U
46	BA	357	U
46	BA	358	G
46	BA	361	C
46	BA	363	A
46	BA	365	A
46	BA	367	A
46	BA	368	G
46	BA	370	A
46	BA	372	U
46	BA	374	U
46	BA	375	A
46	BA	380	A
46	BA	382	C
46	BA	389	A
46	BA	390	A
46	BA	391	U
46	BA	392	A
46	BA	393	C
46	BA	396	C
46	BA	397	A
46	BA	398	A
46	BA	401	A
46	BA	403	C
46	BA	404	C
46	BA	405	U
46	BA	406	A
46	BA	408	A
46	BA	413	A
46	BA	416	G
46	BA	417	U
46	BA	419	U
46	BA	426	G
46	BA	427	A
46	BA	428	G

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Mol	Chain	Res	Type
46	BA	432	G
46	BA	433	U
46	BA	439	A
46	BA	444	A
46	BA	445	C
46	BA	447	G
46	BA	448	C
46	BA	458	A
46	BA	459	C
46	BA	460	G
46	BA	462	A
46	BA	463	U
46	BA	464	A
46	BA	466	A
46	BA	467	A
46	BA	468	C
46	BA	471	U
46	BA	472	G
46	BA	473	A
46	BA	474	C
46	BA	475	U
46	BA	476	A
46	BA	477	G
46	BA	478	A
46	BA	479	G
46	BA	480	A
46	BA	486	U
46	BA	487	C
46	BA	488	U
46	BA	490	A
46	BA	491	A
46	BA	492	U
46	BA	493	A
46	BA	495	U
46	BA	496	A
46	BA	497	C
46	BA	498	C
46	BA	499	A
46	BA	501	A
46	BA	503	U
46	BA	504	A
46	BA	505	G

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Mol	Chain	Res	Type
46	BA	508	C
46	BA	509	U
46	BA	510	A
46	BA	512	A
46	BA	513	A
46	BA	514	G
46	BA	515	C
46	BA	516	A
46	BA	519	C
46	BA	521	U
46	BA	522	C
46	BA	524	A
46	BA	525	U
46	BA	526	U
46	BA	527	G
46	BA	528	A
46	BA	529	G
46	BA	530	A
46	BA	533	G
46	BA	539	A
46	BA	542	C
46	BA	543	U
46	BA	545	A
46	BA	546	A
46	BA	548	A
46	BA	549	A
46	BA	550	A
46	BA	552	U
46	BA	553	C
46	BA	554	A
46	BA	556	C
46	BA	557	A
46	BA	558	A
46	BA	559	C
46	BA	560	A
46	BA	561	U
46	BA	564	U
46	BA	567	C
46	BA	568	A
46	BA	570	A
46	BA	571	A
46	BA	572	A

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Mol	Chain	Res	Type
46	BA	573	C
46	BA	574	U
46	BA	576	A
46	BA	577	U
46	BA	578	A
46	BA	579	A
46	BA	581	A
46	BA	582	A
46	BA	583	A
46	BA	584	C
46	BA	587	C
46	BA	588	U
46	BA	590	G
46	BA	591	C
46	BA	593	C
46	BA	594	A
46	BA	598	C
46	BA	600	G
46	BA	611	U
46	BA	614	A
46	BA	615	A
46	BA	616	A
46	BA	617	C
46	BA	618	A
46	BA	619	U
46	BA	620	A
46	BA	623	A
46	BA	624	G
46	BA	626	A
46	BA	629	A
46	BA	630	A
46	BA	632	G
46	BA	638	A
46	BA	641	A
46	BA	646	C
46	BA	647	A
46	BA	648	A
46	BA	653	C
46	BA	654	C
46	BA	655	U
46	BA	658	C
46	BA	659	U

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Mol	Chain	Res	Type
46	BA	672	U
46	BA	673	U
46	BA	682	A
46	BA	687	A
46	BA	688	U
46	BA	689	A
46	BA	692	A
46	BA	693	U
46	BA	695	C
46	BA	702	U
46	BA	703	U
46	BA	705	A
46	BA	706	C
46	BA	707	A
46	BA	710	C
46	BA	711	A
46	BA	716	A
46	BA	717	C
46	BA	718	C
46	BA	719	A
46	BA	720	A
46	BA	722	A
46	BA	723	C
46	BA	724	A
46	BA	725	A
46	BA	726	C
46	BA	734	C
46	BA	735	G
46	BA	741	U
46	BA	742	A
46	BA	743	A
46	BA	744	U
46	BA	745	U
46	BA	746	A
46	BA	747	C
46	BA	748	A
46	BA	751	G
46	BA	761	C
46	BA	762	A
46	BA	763	C
46	BA	764	A
46	BA	768	G

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Mol	Chain	Res	Type
46	BA	772	A
46	BA	773	C
46	BA	774	C
46	BA	775	A
46	BA	776	A
46	BA	777	G
46	BA	778	G
46	BA	779	A
46	BA	780	A
46	BA	781	A
46	BA	787	A
46	BA	802	A
46	BA	807	G
46	BA	812	C
46	BA	813	A
46	BA	816	A
46	BA	817	A
46	BA	822	G
46	BA	823	C
46	BA	826	G
46	BA	831	C
46	BA	832	C
46	BA	833	A
46	BA	838	C
46	BA	844	C
46	BA	845	U
46	BA	846	C
46	BA	847	U
46	BA	848	A
46	BA	849	G
46	BA	850	C
46	BA	851	A
46	BA	852	U
46	BA	853	U
46	BA	857	A
46	BA	858	G
46	BA	862	U
46	BA	866	G
46	BA	870	A
46	BA	880	A
46	BA	881	G
46	BA	885	C

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Mol	Chain	Res	Type
46	BA	886	A
46	BA	890	G
46	BA	892	U
46	BA	893	U
46	BA	895	A
46	BA	897	G
46	BA	898	G
46	BA	899	C
46	BA	900	C
46	BA	904	G
46	BA	905	U
46	BA	906	A
46	BA	920	A
46	BA	921	A
46	BA	922	G
46	BA	923	G
46	BA	924	U
46	BA	925	A
46	BA	926	G
46	BA	929	U
46	BA	931	A
46	BA	932	U
46	BA	933	C
46	BA	937	U
46	BA	946	A
46	BA	948	U
46	BA	956	U
46	BA	957	G
46	BA	958	U
46	BA	959	A
46	BA	962	A
46	BA	963	A
46	BA	965	G
46	BA	968	C
46	BA	975	G
46	BA	977	G
46	BA	979	U
46	BA	980	U
46	BA	981	U
46	BA	984	U
46	BA	989	C
46	BA	990	U

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Mol	Chain	Res	Type
46	BA	997	C
46	BA	1013	C
46	BA	1014	C
46	BA	1016	U
46	BA	1023	A
46	BA	1025	G
46	BA	1026	A
46	BA	1032	G
46	BA	1036	A
46	BA	1039	A
46	BA	1043	U
46	BA	1048	C
46	BA	1049	G
46	BA	1051	G
46	BA	1052	A
46	BA	1053	A
46	BA	1054	G
46	BA	1055	A
46	BA	1060	A
46	BA	1061	U
46	BA	1062	G
46	BA	1063	G
46	BA	1071	A
46	BA	1073	U
46	BA	1078	A
46	BA	1087	G
46	BA	1088	U
46	BA	1089	U
46	BA	1125	A
46	BA	1127	C
46	BA	1135	A
46	BA	1136	G
46	BA	1138	A
46	BA	1140	U
46	BA	1144	G
46	BA	1147	U
46	BA	1149	G
46	BA	1157	U
46	BA	1161	A
46	BA	1162	G
46	BA	1164	A
46	BA	1165	C

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Mol	Chain	Res	Type
46	BA	1166	A
46	BA	1167	A
46	BA	1176	C
46	BA	1181	U
46	BA	1182	G
46	BA	1184	U
46	BA	1185	U
46	BA	1186	U
46	BA	1187	U
46	BA	1193	A
46	BA	1199	A
46	BA	1204	U
46	BA	1205	C
46	BA	1211	A
46	BA	1224	C
46	BA	1226	U
46	BA	1230	G
46	BA	1232	U
46	BA	1236	A
46	BA	1237	A
46	BA	1238	A
46	BA	1239	U
46	BA	1240	U
46	BA	1241	U
46	BA	1243	G
46	BA	1244	A
46	BA	1245	U
46	BA	1246	C
46	BA	1247	A
46	BA	1249	C
46	BA	1251	G
46	BA	1252	A
46	BA	1262	C
46	BA	1266	G
46	BA	1268	G
46	BA	1269	A
46	BA	1284	U
46	BA	1285	G
46	BA	1286	U
46	BA	1289	U
46	BA	1290	A
46	BA	1292	A

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Mol	Chain	Res	Type
46	BA	1294	U
46	BA	1295	U
46	BA	1297	C
46	BA	1301	C
46	BA	1305	A
46	BA	1306	A
46	BA	1309	G
46	BA	1312	U
46	BA	1313	U
46	BA	1315	A
46	BA	1322	C
46	BA	1323	G
46	BA	1324	A
46	BA	1326	G
46	BA	1327	U
46	BA	1330	G
46	BA	1339	A
46	BA	1340	C
46	BA	1344	A
46	BA	1346	U
46	BA	1347	G
46	BA	1349	U
46	BA	1350	G
46	BA	1351	C
46	BA	1355	C
46	BA	1356	G
46	BA	1375	U
46	BA	1377	C
46	BA	1383	U
46	BA	1385	A
46	BA	1387	A
46	BA	1388	G
46	BA	1394	C
46	BA	1397	G
46	BA	1399	U
46	BA	1402	G
46	BA	1406	U
46	BA	1407	C
46	BA	1411	C
46	BA	1412	C
46	BA	1420	U
46	BA	1423	A

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Mol	Chain	Res	Type
46	BA	1424	G
46	BA	1426	U
46	BA	1427	C
46	BA	1428	G
46	BA	1429	G
46	BA	1430	U
46	BA	1431	U
46	BA	1432	U
46	BA	1433	C
46	BA	1434	U
46	BA	1436	U
46	BA	1443	U
46	BA	1446	A
46	BA	1450	C
46	BA	1451	U
46	BA	1453	C
46	BA	1455	A
46	BA	1456	G
46	BA	1457	U
46	BA	1465	G
46	BA	1466	A
46	BA	1471	A
46	BA	1472	G
46	BA	1474	A
46	BA	1480	A
46	BA	1488	C
46	BA	1489	A
46	BA	1490	C
46	BA	1491	A
46	BA	1492	A
46	BA	1493	A
46	BA	1496	C
46	BA	1501	C
46	BA	1502	A
46	BA	1503	G
46	BA	1506	A
46	BA	1507	U
46	BA	1508	A
46	BA	1510	U
46	BA	1511	U
46	BA	1512	A
46	BA	1516	A

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Mol	Chain	Res	Type
46	BA	1518	U
46	BA	1519	U
46	BA	1520	A
46	BA	1522	U
46	BA	1523	C
46	BA	1524	U
46	BA	1525	U
46	BA	1526	A
46	BA	1529	C
46	BA	1530	U
46	BA	1531	A
46	BA	1532	A
46	BA	1534	U
46	BA	1541	U
46	BA	1542	A
46	BA	1543	A
46	BA	1546	A
46	BA	1547	A
46	BA	1548	U
46	BA	1549	C
46	BA	1550	C
46	BA	1551	A
46	BA	1552	G
46	BA	1556	U
46	BA	1557	A
46	BA	1568	C
46	BA	1569	A
47	BB	7	P5P
47	BB	8	Y5P
47	BB	9	P5P
47	BB	14	P5P
47	BB	15	P5P
47	BB	24	P5P
47	BB	25	P5P
47	BB	34	Y5P
47	BB	35	P5P
47	BB	36	P5P
47	BB	43	Y5P
47	BB	44	Y5P
47	BB	49	P5P

All (37) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	124	A
1	AA	127	A
1	AA	317	A
1	AA	395	C
1	AA	825	C
1	AA	900	A
1	AA	901	A
46	BA	39	A
46	BA	48	U
46	BA	69	C
46	BA	96	U
46	BA	100	C
46	BA	112	A
46	BA	160	A
46	BA	275	G
46	BA	292	U
46	BA	294	G
46	BA	347	G
46	BA	350	A
46	BA	431	A
46	BA	446	A
46	BA	463	U
46	BA	467	A
46	BA	512	A
46	BA	521	U
46	BA	555	C
46	BA	572	A
46	BA	573	C
46	BA	583	A
46	BA	653	C
46	BA	774	C
46	BA	812	C
46	BA	936	U
46	BA	1139	A
46	BA	1423	A
46	BA	1431	U
46	BA	1518	U

5.4 Non-standard residues in protein, DNA, RNA chains (i)

202 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
18	Y5P	AX	12	-	14,16,20	4.30	2 (14%)	19,22,29	1.01	1 (5%)
17	Y5P	AV	1	-	14,16,20	4.63	3 (21%)	19,22,29	1.13	2 (10%)
17	Y5P	AY	1	-	14,16,20	4.65	3 (21%)	19,22,29	1.06	1 (5%)
47	Y5P	BB	6	47	14,19,20	4.24	2 (14%)	18,26,29	0.99	1 (5%)
47	Y5P	BB	40	47	14,19,20	4.22	2 (14%)	18,26,29	1.01	1 (5%)
17	Y5P	AV	12	-	14,19,20	4.30	2 (14%)	18,26,29	1.04	1 (5%)
17	Y5P	AV	67	-	14,19,20	4.63	2 (14%)	18,26,29	1.34	2 (11%)
47	P5P	BB	37	47	20,23,24	0.46	0	27,33,36	0.89	1 (3%)
17	Y5P	AV	52	-	14,19,20	4.66	3 (21%)	18,26,29	1.12	1 (5%)
17	Y5P	AY	37	-	14,19,20	4.67	3 (21%)	18,26,29	1.07	1 (5%)
17	Y5P	AY	29	-	14,19,20	4.65	3 (21%)	18,26,29	1.08	1 (5%)
17	Y5P	AV	13	-	14,19,20	4.55	2 (14%)	18,26,29	1.36	2 (11%)
17	Y5P	AY	30	-	14,19,20	4.65	3 (21%)	18,26,29	1.07	1 (5%)
17	Y5P	AV	66	-	14,19,20	4.40	2 (14%)	18,26,29	1.02	1 (5%)
18	Y5P	AX	17	-	14,19,20	4.17	2 (14%)	18,26,29	0.98	1 (5%)
17	Y5P	AV	49	-	14,19,20	4.62	2 (14%)	18,26,29	1.33	2 (11%)
17	Y5P	AV	24	-	14,19,20	4.66	3 (21%)	18,26,29	1.06	1 (5%)
17	Y5P	AY	33	-	14,19,20	4.25	2 (14%)	18,26,29	1.03	1 (5%)
47	P5P	BB	9	47	20,23,24	0.43	0	27,33,36	0.78	1 (3%)
17	Y5P	AV	45	-	14,19,20	4.44	2 (14%)	18,26,29	0.97	1 (5%)
18	Y5P	AX	22	-	14,19,20	4.36	2 (14%)	18,26,29	1.12	1 (5%)
17	Y5P	AV	29	-	14,19,20	4.60	3 (21%)	18,26,29	1.18	1 (5%)
17	Y5P	AY	73	-	14,19,20	4.73	3 (21%)	18,26,29	1.47	3 (16%)
47	Y5P	BB	11	47	14,19,20	4.68	2 (14%)	18,26,29	1.29	1 (5%)
17	Y5P	AV	65	-	14,19,20	4.66	3 (21%)	18,26,29	1.06	1 (5%)
17	Y5P	AY	51	-	14,19,20	4.30	2 (14%)	18,26,29	1.05	1 (5%)
17	Y5P	AV	33	-	14,19,20	4.32	2 (14%)	18,26,29	0.93	1 (5%)
17	Y5P	AY	65	-	14,19,20	4.67	3 (21%)	18,26,29	1.08	1 (5%)
17	Y5P	AV	68	-	14,19,20	4.61	2 (14%)	18,26,29	1.32	2 (11%)
17	Y5P	AV	2	-	14,19,20	4.72	2 (14%)	18,26,29	1.17	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	Y5P	AV	69	-	14,19,20	4.68	3 (21%)	18,26,29	1.09	1 (5%)
17	Y5P	AV	73	-	14,19,20	4.71	3 (21%)	18,26,29	1.32	3 (16%)
17	Y5P	AY	44	-	14,19,20	4.69	3 (21%)	18,26,29	1.06	1 (5%)
18	Y5P	AX	16	-	14,19,20	4.16	2 (14%)	18,26,29	1.08	1 (5%)
17	Y5P	AV	31	-	14,19,20	4.66	3 (21%)	18,26,29	1.05	1 (5%)
47	P5P	BB	29	47	20,23,24	1.01	2 (10%)	27,33,36	1.91	3 (11%)
17	Y5P	AV	21	-	14,19,20	4.71	3 (21%)	18,26,29	1.15	1 (5%)
17	Y5P	AY	2	-	14,19,20	4.65	2 (14%)	18,26,29	1.27	2 (11%)
17	Y5P	AY	13	-	14,19,20	4.57	2 (14%)	18,26,29	1.37	2 (11%)
17	Y5P	AY	66	-	14,19,20	4.27	2 (14%)	18,26,29	1.05	1 (5%)
17	Y5P	AY	27	-	14,19,20	4.65	3 (21%)	18,26,29	1.21	2 (11%)
17	Y5P	AV	44	-	14,19,20	4.69	3 (21%)	18,26,29	1.09	1 (5%)
47	Y5P	BB	63	47	14,19,20	4.67	2 (14%)	18,26,29	1.28	2 (11%)
47	P5P	BB	36	47	20,23,24	0.48	0	27,33,36	0.80	1 (3%)
17	Y5P	AV	5	-	14,19,20	4.66	3 (21%)	18,26,29	1.05	1 (5%)
17	Y5P	AV	4	-	14,19,20	4.60	2 (14%)	18,26,29	1.29	2 (11%)
17	Y5P	AY	6	-	14,19,20	4.65	3 (21%)	18,26,29	1.07	1 (5%)
17	Y5P	AV	54	-	14,19,20	4.37	2 (14%)	18,26,29	1.02	1 (5%)
17	Y5P	AV	61	-	14,19,20	4.58	2 (14%)	18,26,29	1.33	2 (11%)
17	Y5P	AY	32	-	14,19,20	4.22	2 (14%)	18,26,29	1.00	1 (5%)
17	Y5P	AY	15	-	14,19,20	4.66	3 (21%)	18,26,29	1.14	2 (11%)
17	Y5P	AY	61	-	14,19,20	4.51	2 (14%)	18,26,29	1.42	2 (11%)
47	Y5P	BB	43	47	14,19,20	4.55	2 (14%)	18,26,29	1.43	2 (11%)
17	Y5P	AY	62	-	14,19,20	4.58	2 (14%)	18,26,29	1.40	2 (11%)
17	Y5P	AY	41	-	14,19,20	4.56	2 (14%)	18,26,29	1.42	2 (11%)
47	P5P	BB	25	47	20,23,24	1.04	3 (15%)	27,33,36	1.91	4 (14%)
17	Y5P	AV	27	-	14,19,20	4.71	3 (21%)	18,26,29	1.14	2 (11%)
17	Y5P	AY	43	-	14,19,20	4.55	2 (14%)	18,26,29	1.36	2 (11%)
17	Y5P	AV	23	-	14,19,20	4.65	3 (21%)	18,26,29	1.05	1 (5%)
47	Y5P	BB	34	47	14,19,20	4.42	2 (14%)	18,26,29	1.03	1 (5%)
47	P5P	BB	64	47	20,23,24	0.50	0	27,33,36	0.72	1 (3%)
17	Y5P	AY	60	-	14,19,20	4.27	2 (14%)	18,26,29	1.00	1 (5%)
17	Y5P	AV	9	-	14,19,20	4.65	3 (21%)	18,26,29	1.11	1 (5%)
47	P5P	BB	32	47	20,23,24	0.49	0	27,33,36	0.70	0
17	Y5P	AY	52	-	14,19,20	4.63	3 (21%)	18,26,29	1.13	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	Y5P	AV	10	-	14,19,20	4.64	3 (21%)	18,26,29	1.11	1 (5%)
17	Y5P	AV	25	-	14,19,20	4.71	2 (14%)	18,26,29	1.27	1 (5%)
47	P5P	BB	5	47	20,23,24	0.48	0	27,33,36	0.71	1 (3%)
47	P5P	BB	49	47	20,23,24	1.05	3 (15%)	27,33,36	1.90	4 (14%)
47	P5P	BB	10	47	20,23,24	0.90	2 (10%)	27,33,36	1.91	3 (11%)
17	Y5P	AV	39	-	14,19,20	4.22	2 (14%)	18,26,29	1.07	1 (5%)
17	Y5P	AV	30	-	14,19,20	4.68	3 (21%)	18,26,29	1.09	1 (5%)
17	Y5P	AY	39	-	14,19,20	4.21	2 (14%)	18,26,29	1.04	1 (5%)
47	P5P	BB	7	47	20,23,24	0.97	3 (15%)	27,33,36	1.97	3 (11%)
17	Y5P	AY	53	-	14,19,20	4.65	3 (21%)	18,26,29	1.09	1 (5%)
17	Y5P	AY	4	-	14,19,20	4.66	2 (14%)	18,26,29	1.36	2 (11%)
17	Y5P	AY	12	-	14,19,20	4.24	2 (14%)	18,26,29	1.01	1 (5%)
47	Y5P	BB	53	47	14,19,20	4.59	2 (14%)	18,26,29	1.37	2 (11%)
17	Y5P	AY	70	-	14,19,20	4.68	3 (21%)	18,26,29	1.07	1 (5%)
17	Y5P	AY	10	-	14,19,20	4.64	3 (21%)	18,26,29	1.09	1 (5%)
17	Y5P	AV	53	-	14,19,20	4.65	3 (21%)	18,26,29	1.04	1 (5%)
17	Y5P	AY	14	-	14,19,20	4.65	3 (21%)	18,26,29	1.02	1 (5%)
17	Y5P	AY	28	-	14,19,20	4.66	3 (21%)	18,26,29	1.07	1 (5%)
17	Y5P	AV	26	-	14,19,20	4.66	3 (21%)	18,26,29	1.08	1 (5%)
17	Y5P	AY	63	-	14,19,20	4.63	3 (21%)	18,26,29	1.06	1 (5%)
47	P5P	BB	39	47	20,23,24	0.53	0	27,33,36	0.74	1 (3%)
47	P5P	BB	30	47	20,23,24	1.03	2 (10%)	27,33,36	1.74	4 (14%)
17	P5P	AV	35	-	20,23,24	0.47	0	27,33,36	0.78	1 (3%)
17	Y5P	AY	59	-	14,19,20	4.31	2 (14%)	18,26,29	1.00	1 (5%)
17	P5P	AY	35	-	20,23,24	0.48	0	27,33,36	0.77	1 (3%)
47	Y5P	BB	8	47	14,19,20	4.27	2 (14%)	18,26,29	1.08	1 (5%)
47	Y5P	BB	60	47	14,19,20	4.50	2 (14%)	18,26,29	1.40	2 (11%)
47	P5P	BB	15	47	20,23,24	0.49	0	27,33,36	0.69	1 (3%)
47	Y5P	BB	61	47	14,19,20	4.28	2 (14%)	18,26,29	1.00	1 (5%)
17	Y5P	AY	45	-	14,19,20	4.20	2 (14%)	18,26,29	1.04	1 (5%)
17	Y5P	AV	14	-	14,19,20	4.67	3 (21%)	18,26,29	1.11	1 (5%)
17	Y5P	AY	50	-	14,19,20	4.25	2 (14%)	18,26,29	1.04	1 (5%)
17	Y5P	AY	74	-	14,19,20	4.67	2 (14%)	18,26,29	1.26	2 (11%)
17	Y5P	AY	38	-	14,19,20	4.64	3 (21%)	18,26,29	1.06	1 (5%)
18	Y5P	AX	20	-	14,19,20	4.21	2 (14%)	18,26,29	1.05	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
47	P5P	BB	51	47	20,23,24	0.98	2 (10%)	27,33,36	1.91	4 (14%)
17	Y5P	AY	9	-	14,19,20	4.64	3 (21%)	18,26,29	1.06	1 (5%)
47	P5P	BB	45	47	20,23,24	0.47	0	27,33,36	0.71	0
17	Y5P	AV	38	-	14,19,20	4.64	3 (21%)	18,26,29	1.05	1 (5%)
17	Y5P	AY	22	-	14,19,20	4.65	3 (21%)	18,26,29	1.08	1 (5%)
17	Y5P	AY	40	-	14,19,20	4.48	2 (14%)	18,26,29	1.43	2 (11%)
47	Y5P	BB	33	47	14,19,20	4.56	2 (14%)	18,26,29	1.37	2 (11%)
17	Y5P	AY	49	-	14,19,20	4.49	2 (14%)	18,26,29	1.40	2 (11%)
17	Y5P	AV	50	-	14,19,20	4.40	2 (14%)	18,26,29	0.99	1 (5%)
18	Y5P	AX	21	-	14,19,20	4.57	2 (14%)	18,26,29	1.41	2 (11%)
17	Y5P	AV	22	-	14,19,20	4.67	3 (21%)	18,26,29	1.09	1 (5%)
17	Y5P	AV	72	-	14,19,20	4.67	2 (14%)	18,26,29	1.33	1 (5%)
17	Y5P	AY	72	-	14,19,20	4.70	2 (14%)	18,26,29	1.26	1 (5%)
47	Y5P	BB	31	47	14,19,20	4.63	2 (14%)	18,26,29	1.35	2 (11%)
17	Y5P	AV	6	-	14,19,20	4.65	3 (21%)	18,26,29	1.04	1 (5%)
17	Y5P	AV	43	-	14,19,20	4.72	2 (14%)	18,26,29	1.24	2 (11%)
47	P5P	BB	38	47	20,23,24	0.54	0	27,33,36	0.77	1 (3%)
18	Y5P	AX	14	-	14,19,20	4.42	2 (14%)	18,26,29	0.97	1 (5%)
47	P5P	BB	27	47	20,23,24	0.48	0	27,33,36	0.85	0
17	Y5P	AV	51	-	14,19,20	4.38	2 (14%)	18,26,29	1.00	1 (5%)
17	P5P	AV	36	-	20,23,24	0.48	0	27,33,36	0.74	1 (3%)
47	P5P	BB	46	47	20,23,24	0.93	3 (15%)	27,33,36	1.83	3 (11%)
17	Y5P	AY	11	-	14,19,20	4.58	2 (14%)	18,26,29	1.35	2 (11%)
17	Y5P	AY	71	-	14,19,20	4.67	3 (21%)	18,26,29	1.14	1 (5%)
17	Y5P	AY	5	-	14,19,20	4.65	3 (21%)	18,26,29	1.10	1 (5%)
47	Y5P	BB	62	47	14,19,20	4.33	2 (14%)	18,26,29	1.01	1 (5%)
18	Y5P	AX	23	-	14,19,20	4.33	2 (14%)	18,26,29	1.02	1 (5%)
47	P5P	BB	35	47	20,23,24	1.11	3 (15%)	27,33,36	1.87	3 (11%)
47	Y5P	BB	44	47	14,19,20	4.26	2 (14%)	18,26,29	0.96	1 (5%)
17	Y5P	AV	11	-	14,19,20	4.50	2 (14%)	18,26,29	1.44	2 (11%)
47	P5P	BB	14	47	20,23,24	0.48	0	27,33,36	0.79	1 (3%)
17	Y5P	AV	48	-	14,19,20	4.56	2 (14%)	18,26,29	1.49	2 (11%)
17	Y5P	AY	7	-	14,19,20	4.65	3 (21%)	18,26,29	1.05	1 (5%)
17	Y5P	AY	55	-	14,19,20	4.42	2 (14%)	18,26,29	1.14	2 (11%)
47	Y5P	BB	12	47	14,19,20	4.31	2 (14%)	18,26,29	0.99	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	Y5P	AV	71	-	14,19,20	4.65	3 (21%)	18,26,29	1.05	1 (5%)
17	P5P	AY	34	-	20,23,24	1.00	2 (10%)	27,33,36	2.00	3 (11%)
17	P5P	AY	36	-	20,23,24	0.54	0	27,33,36	0.80	1 (3%)
17	Y5P	AV	8	-	14,19,20	4.12	2 (14%)	18,26,29	1.13	1 (5%)
17	Y5P	AY	25	-	14,19,20	4.54	2 (14%)	18,26,29	1.34	2 (11%)
47	P5P	BB	41	47	20,23,24	1.00	2 (10%)	27,33,36	1.95	4 (14%)
17	Y5P	AV	7	-	14,19,20	4.61	3 (21%)	18,26,29	1.03	1 (5%)
17	Y5P	AY	8	-	14,19,20	4.23	2 (14%)	18,26,29	1.03	1 (5%)
17	Y5P	AV	40	-	14,19,20	4.63	2 (14%)	18,26,29	1.34	2 (11%)
17	Y5P	AV	55	-	14,19,20	4.30	2 (14%)	18,26,29	1.06	1 (5%)
17	Y5P	AY	67	-	14,19,20	4.63	2 (14%)	18,26,29	1.40	1 (5%)
17	Y5P	AY	3	-	14,19,20	4.50	2 (14%)	18,26,29	1.43	2 (11%)
47	P5P	BB	58	47	20,23,24	0.49	0	27,33,36	0.70	1 (3%)
17	Y5P	AV	59	-	14,19,20	4.32	2 (14%)	18,26,29	1.00	1 (5%)
18	Y5P	AX	15	-	14,19,20	4.43	2 (14%)	18,26,29	1.06	1 (5%)
17	Y5P	AV	58	-	14,19,20	4.67	3 (21%)	18,26,29	1.12	1 (5%)
18	Y5P	AX	24	-	14,19,20	4.51	2 (14%)	18,26,29	0.94	1 (5%)
17	Y5P	AV	74	-	14,19,20	4.70	2 (14%)	18,26,29	1.21	2 (11%)
17	Y5P	AY	48	-	14,19,20	4.53	2 (14%)	18,26,29	1.36	2 (11%)
47	Y5P	BB	42	47	14,19,20	4.54	2 (14%)	18,26,29	1.44	2 (11%)
17	Y5P	AY	31	-	14,19,20	4.65	3 (21%)	18,26,29	1.04	1 (5%)
17	Y5P	AY	75	-	14,19,20	4.59	2 (14%)	18,26,29	1.34	2 (11%)
47	Y5P	BB	48	47	14,19,20	4.28	2 (14%)	18,26,29	1.03	1 (5%)
17	Y5P	AY	21	-	14,19,20	4.65	3 (21%)	18,26,29	1.07	1 (5%)
47	P5P	BB	24	47	20,23,24	0.46	0	27,33,36	0.84	0
47	Y5P	BB	13	47	14,19,20	4.20	2 (14%)	18,26,29	1.23	1 (5%)
17	Y5P	AV	63	-	14,19,20	4.67	3 (21%)	18,26,29	1.06	1 (5%)
17	Y5P	AV	62	-	14,19,20	4.52	2 (14%)	18,26,29	1.38	2 (11%)
17	Y5P	AV	41	-	14,19,20	4.63	2 (14%)	18,26,29	1.37	2 (11%)
47	Y5P	BB	26	47	14,19,20	4.55	2 (14%)	18,26,29	1.40	2 (11%)
17	Y5P	AY	24	-	14,19,20	4.64	3 (21%)	18,26,29	1.04	1 (5%)
17	Y5P	AV	37	-	14,19,20	4.67	3 (21%)	18,26,29	1.07	1 (5%)
18	Y5P	AX	19	-	14,19,20	4.28	2 (14%)	18,26,29	0.95	1 (5%)
17	Y5P	AY	68	-	14,19,20	4.58	2 (14%)	18,26,29	1.30	2 (11%)
17	Y5P	AV	56	-	14,19,20	4.61	2 (14%)	18,26,29	1.30	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
47	Y5P	BB	52	47	14,19,20	4.61	2 (14%)	18,26,29	1.34	2 (11%)
17	Y5P	AY	56	-	14,19,20	4.58	2 (14%)	18,26,29	1.33	2 (11%)
47	P5P	BB	47	47	20,23,24	0.40	0	27,33,36	0.90	2 (7%)
17	Y5P	AV	75	-	14,19,20	4.37	2 (14%)	18,26,29	1.43	2 (11%)
17	Y5P	AV	60	-	14,19,20	4.34	2 (14%)	18,26,29	1.08	1 (5%)
17	P5P	AY	76	46	20,23,24	0.60	1 (5%)	27,33,36	0.74	1 (3%)
17	Y5P	AY	23	-	14,19,20	4.67	3 (21%)	18,26,29	1.03	1 (5%)
47	P5P	BB	59	47	20,23,24	1.01	3 (15%)	27,33,36	1.86	4 (14%)
18	Y5P	AX	18	-	14,19,20	4.54	2 (14%)	18,26,29	1.30	2 (11%)
17	Y5P	AY	58	-	14,19,20	4.64	3 (21%)	18,26,29	1.12	1 (5%)
17	Y5P	AY	69	-	14,19,20	4.67	3 (21%)	18,26,29	1.22	2 (11%)
17	Y5P	AY	57	-	14,19,20	4.67	3 (21%)	18,26,29	1.03	1 (5%)
17	P5P	AV	76	46	20,23,24	0.54	0	27,33,36	0.81	1 (3%)
17	P5P	AV	34	-	20,23,24	1.13	3 (15%)	27,33,36	2.00	4 (14%)
17	Y5P	AV	57	-	14,19,20	4.73	3 (21%)	18,26,29	1.12	1 (5%)
17	Y5P	AY	64	-	14,19,20	4.68	3 (21%)	18,26,29	1.11	1 (5%)
47	Y5P	BB	65	47	14,19,20	4.19	2 (14%)	18,26,29	1.09	1 (5%)
47	P5P	BB	28	47	20,23,24	0.49	0	27,33,36	0.72	1 (3%)
17	Y5P	AY	26	-	14,19,20	4.70	3 (21%)	18,26,29	1.05	1 (5%)
47	P5P	BB	23	47	20,23,24	0.55	0	27,33,36	1.33	4 (14%)
17	Y5P	AY	42	-	14,19,20	4.58	2 (14%)	18,26,29	1.47	2 (11%)
17	Y5P	AV	3	-	14,19,20	4.70	2 (14%)	18,26,29	1.28	2 (11%)
18	Y5P	AX	13	-	14,19,20	4.34	2 (14%)	18,26,29	1.02	1 (5%)
17	Y5P	AV	64	-	14,19,20	4.69	3 (21%)	18,26,29	1.04	1 (5%)
17	Y5P	AY	54	-	14,19,20	4.25	2 (14%)	18,26,29	1.05	1 (5%)
47	P5P	BB	50	47	20,23,24	0.51	0	27,33,36	0.77	0
17	Y5P	AV	32	-	14,19,20	4.34	2 (14%)	18,26,29	1.00	1 (5%)
17	Y5P	AV	15	-	14,19,20	4.63	3 (21%)	18,26,29	1.03	1 (5%)
17	Y5P	AV	42	-	14,19,20	4.63	2 (14%)	18,26,29	1.27	2 (11%)
17	Y5P	AV	70	-	14,19,20	4.67	3 (21%)	18,26,29	1.07	1 (5%)
17	Y5P	AV	28	-	14,19,20	4.63	3 (21%)	18,26,29	1.03	1 (5%)
47	P5P	BB	66	47	20,23,24	0.45	0	27,33,36	0.74	1 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	Y5P	AX	12	-	-	3/6/30/34	0/2/2/2
17	Y5P	AV	1	-	-	1/6/30/34	0/2/2/2
17	Y5P	AY	1	-	-	1/6/30/34	0/2/2/2
47	Y5P	BB	6	47	-	1/7/33/34	0/2/2/2
47	Y5P	BB	40	47	-	1/7/33/34	0/2/2/2
17	Y5P	AV	12	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	67	-	-	1/7/33/34	0/2/2/2
47	P5P	BB	37	47	-	0/7/25/26	0/3/3/3
17	Y5P	AV	52	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	37	-	-	4/7/33/34	0/2/2/2
17	Y5P	AY	29	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	13	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	30	-	-	4/7/33/34	0/2/2/2
17	Y5P	AV	66	-	-	1/7/33/34	0/2/2/2
18	Y5P	AX	17	-	-	2/7/33/34	0/2/2/2
17	Y5P	AV	49	-	-	3/7/33/34	0/2/2/2
17	Y5P	AV	24	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	33	-	-	1/7/33/34	0/2/2/2
47	P5P	BB	9	47	-	4/7/25/26	0/3/3/3
17	Y5P	AV	45	-	-	1/7/33/34	0/2/2/2
18	Y5P	AX	22	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	29	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	73	-	-	2/7/33/34	0/2/2/2
47	Y5P	BB	11	47	-	1/7/33/34	0/2/2/2
17	Y5P	AV	65	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	51	-	-	3/7/33/34	0/2/2/2
17	Y5P	AV	33	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	65	-	-	3/7/33/34	0/2/2/2
17	Y5P	AV	68	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	2	-	-	3/7/33/34	0/2/2/2
17	Y5P	AV	69	-	-	3/7/33/34	0/2/2/2
17	Y5P	AV	73	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	44	-	-	1/7/33/34	0/2/2/2
18	Y5P	AX	16	-	-	3/7/33/34	0/2/2/2
17	Y5P	AV	31	-	-	1/7/33/34	0/2/2/2
47	P5P	BB	29	47	-	0/7/25/26	0/3/3/3
17	Y5P	AV	21	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	2	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	13	-	-	3/7/33/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	Y5P	AY	66	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	27	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	44	-	-	1/7/33/34	0/2/2/2
47	Y5P	BB	63	47	-	1/7/33/34	0/2/2/2
47	P5P	BB	36	47	-	0/7/25/26	0/3/3/3
17	Y5P	AV	5	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	4	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	6	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	54	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	61	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	32	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	15	-	-	3/7/33/34	0/2/2/2
17	Y5P	AY	61	-	-	3/7/33/34	0/2/2/2
47	Y5P	BB	43	47	-	3/7/33/34	0/2/2/2
17	Y5P	AY	62	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	41	-	-	3/7/33/34	0/2/2/2
47	P5P	BB	25	47	-	2/7/25/26	0/3/3/3
17	Y5P	AV	27	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	43	-	-	4/7/33/34	0/2/2/2
17	Y5P	AV	23	-	-	1/7/33/34	0/2/2/2
47	Y5P	BB	34	47	-	3/7/33/34	0/2/2/2
47	P5P	BB	64	47	-	0/7/25/26	0/3/3/3
17	Y5P	AY	60	-	-	2/7/33/34	0/2/2/2
17	Y5P	AV	9	-	-	5/7/33/34	0/2/2/2
47	P5P	BB	32	47	-	0/7/25/26	0/3/3/3
17	Y5P	AY	52	-	-	2/7/33/34	0/2/2/2
17	Y5P	AV	10	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	25	-	-	1/7/33/34	0/2/2/2
47	P5P	BB	5	47	-	3/7/25/26	0/3/3/3
47	P5P	BB	49	47	-	2/7/25/26	0/3/3/3
47	P5P	BB	10	47	-	0/7/25/26	0/3/3/3
17	Y5P	AV	39	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	30	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	39	-	-	1/7/33/34	0/2/2/2
47	P5P	BB	7	47	-	1/7/25/26	0/3/3/3
17	Y5P	AY	53	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	4	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	12	-	-	1/7/33/34	0/2/2/2
47	Y5P	BB	53	47	-	1/7/33/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	Y5P	AY	70	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	10	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	53	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	14	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	28	-	-	2/7/33/34	0/2/2/2
17	Y5P	AV	26	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	63	-	-	1/7/33/34	0/2/2/2
47	P5P	BB	39	47	-	0/7/25/26	0/3/3/3
47	P5P	BB	30	47	-	0/7/25/26	0/3/3/3
17	P5P	AV	35	-	-	0/7/25/26	0/3/3/3
17	Y5P	AY	59	-	-	2/7/33/34	0/2/2/2
17	P5P	AY	35	-	-	0/7/25/26	0/3/3/3
47	Y5P	BB	8	47	-	2/7/33/34	0/2/2/2
47	Y5P	BB	60	47	-	1/7/33/34	0/2/2/2
47	P5P	BB	15	47	-	2/7/25/26	0/3/3/3
47	Y5P	BB	61	47	-	1/7/33/34	0/2/2/2
17	Y5P	AY	45	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	14	-	-	5/7/33/34	0/2/2/2
17	Y5P	AY	50	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	74	-	-	2/7/33/34	0/2/2/2
17	Y5P	AY	38	-	-	1/7/33/34	0/2/2/2
18	Y5P	AX	20	-	-	1/7/33/34	0/2/2/2
47	P5P	BB	51	47	-	0/7/25/26	0/3/3/3
17	Y5P	AY	9	-	-	3/7/33/34	0/2/2/2
47	P5P	BB	45	47	-	0/7/25/26	0/3/3/3
17	Y5P	AV	38	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	22	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	40	-	-	1/7/33/34	0/2/2/2
47	Y5P	BB	33	47	-	1/7/33/34	0/2/2/2
17	Y5P	AY	49	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	50	-	-	1/7/33/34	0/2/2/2
18	Y5P	AX	21	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	22	-	-	3/7/33/34	0/2/2/2
17	Y5P	AV	72	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	72	-	-	1/7/33/34	0/2/2/2
47	Y5P	BB	31	47	-	1/7/33/34	0/2/2/2
17	Y5P	AV	6	-	-	4/7/33/34	0/2/2/2
17	Y5P	AV	43	-	-	1/7/33/34	0/2/2/2
47	P5P	BB	38	47	-	0/7/25/26	0/3/3/3
18	Y5P	AX	14	-	-	2/7/33/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	P5P	BB	27	47	-	1/7/25/26	0/3/3/3
17	Y5P	AV	51	-	-	1/7/33/34	0/2/2/2
17	P5P	AV	36	-	-	0/7/25/26	0/3/3/3
47	P5P	BB	46	47	-	3/7/25/26	0/3/3/3
17	Y5P	AY	11	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	71	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	5	-	-	1/7/33/34	0/2/2/2
47	Y5P	BB	62	47	-	1/7/33/34	0/2/2/2
18	Y5P	AX	23	-	-	3/7/33/34	0/2/2/2
47	P5P	BB	35	47	-	2/7/25/26	0/3/3/3
47	Y5P	BB	44	47	-	3/7/33/34	0/2/2/2
17	Y5P	AV	11	-	-	1/7/33/34	0/2/2/2
47	P5P	BB	14	47	-	2/7/25/26	0/3/3/3
17	Y5P	AV	48	-	-	3/7/33/34	0/2/2/2
17	Y5P	AY	7	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	55	-	-	2/7/33/34	0/2/2/2
47	Y5P	BB	12	47	-	3/7/33/34	0/2/2/2
17	Y5P	AV	71	-	-	1/7/33/34	0/2/2/2
17	P5P	AY	34	-	-	2/7/25/26	0/3/3/3
17	P5P	AY	36	-	-	0/7/25/26	0/3/3/3
17	Y5P	AV	8	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	25	-	-	1/7/33/34	0/2/2/2
47	P5P	BB	41	47	-	0/7/25/26	0/3/3/3
17	Y5P	AV	7	-	-	3/7/33/34	0/2/2/2
17	Y5P	AY	8	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	40	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	55	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	67	-	-	3/7/33/34	0/2/2/2
17	Y5P	AY	3	-	-	1/7/33/34	0/2/2/2
47	P5P	BB	58	47	-	0/7/25/26	0/3/3/3
17	Y5P	AV	59	-	-	3/7/33/34	0/2/2/2
18	Y5P	AX	15	-	-	3/7/33/34	0/2/2/2
17	Y5P	AV	58	-	-	4/7/33/34	0/2/2/2
18	Y5P	AX	24	-	-	2/7/33/34	0/2/2/2
17	Y5P	AV	74	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	48	-	-	1/7/33/34	0/2/2/2
47	Y5P	BB	42	47	-	1/7/33/34	0/2/2/2
17	Y5P	AY	31	-	-	1/7/33/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	Y5P	AY	75	-	-	2/7/33/34	0/2/2/2
47	Y5P	BB	48	47	-	3/7/33/34	0/2/2/2
17	Y5P	AY	21	-	-	3/7/33/34	0/2/2/2
47	P5P	BB	24	47	-	2/7/25/26	0/3/3/3
47	Y5P	BB	13	47	-	1/7/33/34	0/2/2/2
17	Y5P	AV	63	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	62	-	-	2/7/33/34	0/2/2/2
17	Y5P	AV	41	-	-	1/7/33/34	0/2/2/2
47	Y5P	BB	26	47	-	1/7/33/34	0/2/2/2
17	Y5P	AY	24	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	37	-	-	2/7/33/34	0/2/2/2
18	Y5P	AX	19	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	68	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	56	-	-	1/7/33/34	0/2/2/2
47	Y5P	BB	52	47	-	1/7/33/34	0/2/2/2
17	Y5P	AY	56	-	-	1/7/33/34	0/2/2/2
47	P5P	BB	47	47	-	0/7/25/26	0/3/3/3
17	Y5P	AV	75	-	-	3/7/33/34	0/2/2/2
17	Y5P	AV	60	-	-	1/7/33/34	0/2/2/2
17	P5P	AY	76	46	-	0/7/25/26	0/3/3/3
17	Y5P	AY	23	-	-	2/7/33/34	0/2/2/2
47	P5P	BB	59	47	-	0/7/25/26	0/3/3/3
18	Y5P	AX	18	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	58	-	-	4/7/33/34	0/2/2/2
17	Y5P	AY	69	-	-	2/7/33/34	0/2/2/2
17	Y5P	AY	57	-	-	1/7/33/34	0/2/2/2
17	P5P	AV	76	46	-	1/7/25/26	0/3/3/3
17	P5P	AV	34	-	-	0/7/25/26	0/3/3/3
17	Y5P	AV	57	-	-	2/7/33/34	0/2/2/2
17	Y5P	AY	64	-	-	1/7/33/34	0/2/2/2
47	Y5P	BB	65	47	-	1/7/33/34	0/2/2/2
47	P5P	BB	28	47	-	0/7/25/26	0/3/3/3
17	Y5P	AY	26	-	-	1/7/33/34	0/2/2/2
47	P5P	BB	23	47	-	2/7/25/26	0/3/3/3
17	Y5P	AY	42	-	-	3/7/33/34	0/2/2/2
17	Y5P	AV	3	-	-	1/7/33/34	0/2/2/2
18	Y5P	AX	13	-	-	3/7/33/34	0/2/2/2
17	Y5P	AV	64	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	54	-	-	1/7/33/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	P5P	BB	50	47	-	0/7/25/26	0/3/3/3
17	Y5P	AV	32	-	-	3/7/33/34	0/2/2/2
17	Y5P	AV	15	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	42	-	-	3/7/33/34	0/2/2/2
17	Y5P	AV	70	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	28	-	-	1/7/33/34	0/2/2/2
47	P5P	BB	66	47	-	0/7/25/26	0/3/3/3

All (426) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	AX	24	Y5P	C2-N3	14.77	1.38	1.27
18	AX	15	Y5P	C2-N3	14.73	1.38	1.27
17	AV	69	Y5P	C2-N3	14.48	1.38	1.27
17	AV	63	Y5P	C2-N3	14.48	1.38	1.27
17	AV	57	Y5P	C2-N3	14.47	1.38	1.27
17	AV	73	Y5P	C2-N3	14.46	1.38	1.27
17	AV	9	Y5P	C2-N3	14.46	1.38	1.27
17	AV	23	Y5P	C2-N3	14.45	1.38	1.27
17	AV	52	Y5P	C2-N3	14.45	1.38	1.27
17	AY	69	Y5P	C2-N3	14.45	1.38	1.27
17	AY	5	Y5P	C2-N3	14.45	1.38	1.27
17	AY	29	Y5P	C2-N3	14.44	1.38	1.27
17	AY	73	Y5P	C2-N3	14.44	1.38	1.27
17	AY	23	Y5P	C2-N3	14.44	1.38	1.27
17	AY	57	Y5P	C2-N3	14.44	1.38	1.27
17	AV	30	Y5P	C2-N3	14.43	1.38	1.27
17	AV	27	Y5P	C2-N3	14.43	1.38	1.27
17	AY	10	Y5P	C2-N3	14.43	1.38	1.27
17	AY	28	Y5P	C2-N3	14.43	1.38	1.27
17	AV	44	Y5P	C2-N3	14.43	1.38	1.27
17	AY	44	Y5P	C2-N3	14.43	1.38	1.27
17	AV	29	Y5P	C2-N3	14.42	1.38	1.27
17	AV	1	Y5P	C2-N3	14.42	1.38	1.27
17	AV	22	Y5P	C2-N3	14.42	1.38	1.27
17	AY	15	Y5P	C2-N3	14.41	1.38	1.27
17	AY	14	Y5P	C2-N3	14.41	1.38	1.27
17	AY	22	Y5P	C2-N3	14.41	1.38	1.27
17	AV	71	Y5P	C2-N3	14.41	1.38	1.27
17	AY	26	Y5P	C2-N3	14.41	1.38	1.27
17	AV	65	Y5P	C2-N3	14.41	1.38	1.27
17	AV	6	Y5P	C2-N3	14.41	1.38	1.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	AY	7	Y5P	C2-N3	14.40	1.38	1.27
17	AV	24	Y5P	C2-N3	14.40	1.38	1.27
17	AY	53	Y5P	C2-N3	14.40	1.38	1.27
17	AY	6	Y5P	C2-N3	14.40	1.38	1.27
17	AV	37	Y5P	C2-N3	14.40	1.38	1.27
17	AV	53	Y5P	C2-N3	14.40	1.38	1.27
17	AV	10	Y5P	C2-N3	14.40	1.38	1.27
17	AV	7	Y5P	C2-N3	14.39	1.38	1.27
17	AV	38	Y5P	C2-N3	14.39	1.38	1.27
17	AY	64	Y5P	C2-N3	14.39	1.38	1.27
18	AX	14	Y5P	C2-N3	14.39	1.38	1.27
17	AV	31	Y5P	C2-N3	14.38	1.38	1.27
17	AV	58	Y5P	C2-N3	14.38	1.38	1.27
17	AY	9	Y5P	C2-N3	14.38	1.38	1.27
17	AY	30	Y5P	C2-N3	14.38	1.38	1.27
17	AV	45	Y5P	C2-N3	14.38	1.38	1.27
17	AV	21	Y5P	C2-N3	14.38	1.38	1.27
17	AY	71	Y5P	C2-N3	14.38	1.38	1.27
17	AY	37	Y5P	C2-N3	14.36	1.38	1.27
17	AV	64	Y5P	C2-N3	14.36	1.38	1.27
17	AY	52	Y5P	C2-N3	14.36	1.38	1.27
17	AY	70	Y5P	C2-N3	14.36	1.38	1.27
47	BB	34	Y5P	C2-N3	14.36	1.38	1.27
17	AY	58	Y5P	C2-N3	14.35	1.38	1.27
17	AV	70	Y5P	C2-N3	14.35	1.38	1.27
17	AV	15	Y5P	C2-N3	14.34	1.38	1.27
17	AY	27	Y5P	C2-N3	14.34	1.38	1.27
17	AY	65	Y5P	C2-N3	14.33	1.38	1.27
17	AV	26	Y5P	C2-N3	14.33	1.38	1.27
17	AY	24	Y5P	C2-N3	14.33	1.38	1.27
17	AY	21	Y5P	C2-N3	14.32	1.38	1.27
17	AY	31	Y5P	C2-N3	14.32	1.38	1.27
17	AV	28	Y5P	C2-N3	14.31	1.38	1.27
17	AY	38	Y5P	C2-N3	14.31	1.38	1.27
17	AV	5	Y5P	C2-N3	14.31	1.38	1.27
17	AY	1	Y5P	C2-N3	14.31	1.38	1.27
17	AV	14	Y5P	C2-N3	14.29	1.38	1.27
17	AY	63	Y5P	C2-N3	14.28	1.38	1.27
17	AV	50	Y5P	C2-N3	14.27	1.38	1.27
17	AV	66	Y5P	C2-N3	14.27	1.38	1.27
18	AX	22	Y5P	C2-N3	14.21	1.38	1.27
17	AV	54	Y5P	C2-N3	14.20	1.38	1.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	AX	23	Y5P	C2-N3	14.20	1.38	1.27
17	AV	51	Y5P	C2-N3	14.16	1.38	1.27
17	AV	12	Y5P	C2-N3	14.11	1.38	1.27
17	AV	41	Y5P	C4-N3	-14.05	1.33	1.46
47	BB	12	Y5P	C2-N3	14.03	1.38	1.27
47	BB	62	Y5P	C2-N3	14.02	1.38	1.27
18	AX	12	Y5P	C2-N3	14.01	1.38	1.27
18	AX	13	Y5P	C2-N3	13.98	1.38	1.27
17	AY	51	Y5P	C2-N3	13.96	1.38	1.27
17	AY	55	Y5P	C2-N3	13.87	1.38	1.27
17	AV	32	Y5P	C2-N3	13.86	1.38	1.27
47	BB	61	Y5P	C2-N3	13.86	1.38	1.27
17	AV	60	Y5P	C2-N3	13.85	1.38	1.27
17	AY	59	Y5P	C2-N3	13.82	1.38	1.27
47	BB	48	Y5P	C2-N3	13.82	1.38	1.27
18	AX	21	Y5P	C4-N3	-13.77	1.33	1.46
17	AV	59	Y5P	C2-N3	13.77	1.38	1.27
17	AV	42	Y5P	C4-N3	-13.76	1.33	1.46
47	BB	8	Y5P	C2-N3	13.73	1.38	1.27
17	AY	54	Y5P	C2-N3	13.73	1.38	1.27
17	AV	55	Y5P	C2-N3	13.72	1.38	1.27
17	AY	60	Y5P	C2-N3	13.72	1.38	1.27
17	AY	66	Y5P	C2-N3	13.65	1.38	1.27
17	AV	2	Y5P	C4-N3	-13.61	1.33	1.46
47	BB	31	Y5P	C4-N3	-13.56	1.33	1.46
17	AY	8	Y5P	C2-N3	13.55	1.37	1.27
47	BB	13	Y5P	C2-N3	13.55	1.37	1.27
47	BB	33	Y5P	C4-N3	-13.52	1.33	1.46
47	BB	11	Y5P	C4-N3	-13.51	1.33	1.46
17	AY	12	Y5P	C2-N3	13.50	1.37	1.27
18	AX	19	Y5P	C2-N3	13.47	1.37	1.27
17	AV	40	Y5P	C4-N3	-13.47	1.33	1.46
17	AV	48	Y5P	C4-N3	-13.45	1.33	1.46
17	AY	40	Y5P	C4-N3	-13.40	1.33	1.46
17	AY	39	Y5P	C2-N3	13.38	1.37	1.27
17	AY	50	Y5P	C2-N3	13.38	1.37	1.27
47	BB	6	Y5P	C2-N3	13.37	1.37	1.27
17	AV	3	Y5P	C4-N3	-13.36	1.33	1.46
47	BB	44	Y5P	C2-N3	13.35	1.37	1.27
17	AV	4	Y5P	C4-N3	-13.32	1.33	1.46
17	AV	75	Y5P	C4-N3	-13.31	1.33	1.46
47	BB	63	Y5P	C4-N3	-13.26	1.33	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	AY	48	Y5P	C4-N3	-13.25	1.33	1.46
17	AY	25	Y5P	C4-N3	-13.25	1.33	1.46
17	AY	67	Y5P	C4-N3	-13.25	1.33	1.46
17	AY	41	Y5P	C4-N3	-13.25	1.33	1.46
17	AV	39	Y5P	C2-N3	13.24	1.37	1.27
17	AY	61	Y5P	C4-N3	-13.23	1.33	1.46
18	AX	18	Y5P	C4-N3	-13.22	1.33	1.46
18	AX	20	Y5P	C2-N3	13.20	1.37	1.27
47	BB	53	Y5P	C4-N3	-13.19	1.33	1.46
47	BB	40	Y5P	C2-N3	13.19	1.37	1.27
47	BB	52	Y5P	C4-N3	-13.17	1.33	1.46
17	AV	43	Y5P	C4-N3	-13.16	1.33	1.46
17	AV	72	Y5P	C4-N3	-13.16	1.33	1.46
17	AY	32	Y5P	C2-N3	13.15	1.37	1.27
47	BB	65	Y5P	C2-N3	13.14	1.37	1.27
47	BB	42	Y5P	C4-N3	-13.13	1.33	1.46
17	AV	61	Y5P	C4-N3	-13.13	1.33	1.46
17	AY	62	Y5P	C4-N3	-13.10	1.33	1.46
17	AV	68	Y5P	C4-N3	-13.09	1.33	1.46
18	AX	16	Y5P	C2-N3	13.09	1.37	1.27
17	AV	25	Y5P	C4-N3	-13.09	1.33	1.46
17	AY	43	Y5P	C4-N3	-13.07	1.34	1.46
17	AY	11	Y5P	C4-N3	-13.05	1.34	1.46
47	BB	26	Y5P	C4-N3	-13.05	1.34	1.46
17	AY	45	Y5P	C2-N3	13.05	1.37	1.27
17	AV	67	Y5P	C4-N3	-13.03	1.34	1.46
17	AV	62	Y5P	C4-N3	-13.02	1.34	1.46
17	AY	4	Y5P	C4-N3	-12.97	1.34	1.46
17	AY	33	Y5P	C2-N3	12.97	1.37	1.27
17	AY	72	Y5P	C4-N3	-12.95	1.34	1.46
17	AY	42	Y5P	C4-N3	-12.93	1.34	1.46
17	AV	8	Y5P	C2-N3	12.93	1.37	1.27
17	AY	56	Y5P	C4-N3	-12.91	1.34	1.46
17	AY	49	Y5P	C4-N3	-12.90	1.34	1.46
17	AY	13	Y5P	C4-N3	-12.88	1.34	1.46
47	BB	43	Y5P	C4-N3	-12.87	1.34	1.46
17	AV	33	Y5P	C2-N3	12.87	1.37	1.27
17	AV	74	Y5P	C4-N3	-12.87	1.34	1.46
17	AV	56	Y5P	C4-N3	-12.86	1.34	1.46
17	AY	68	Y5P	C4-N3	-12.80	1.34	1.46
17	AY	75	Y5P	C4-N3	-12.79	1.34	1.46
18	AX	17	Y5P	C2-N3	12.77	1.37	1.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	AV	11	Y5P	C4-N3	-12.77	1.34	1.46
17	AY	3	Y5P	C4-N3	-12.68	1.34	1.46
17	AY	74	Y5P	C4-N3	-12.67	1.34	1.46
17	AV	49	Y5P	C4-N3	-12.65	1.34	1.46
47	BB	60	Y5P	C4-N3	-12.64	1.34	1.46
17	AY	2	Y5P	C4-N3	-12.57	1.34	1.46
17	AV	13	Y5P	C4-N3	-12.32	1.34	1.46
17	AY	74	Y5P	C2-N3	11.96	1.36	1.27
17	AY	2	Y5P	C2-N3	11.95	1.36	1.27
17	AV	74	Y5P	C2-N3	11.89	1.36	1.27
17	AY	72	Y5P	C2-N3	11.77	1.36	1.27
17	AV	13	Y5P	C2-N3	11.69	1.36	1.27
17	AV	49	Y5P	C2-N3	11.68	1.36	1.27
17	AV	43	Y5P	C2-N3	11.68	1.36	1.27
17	AV	25	Y5P	C2-N3	11.67	1.36	1.27
17	AY	4	Y5P	C2-N3	11.58	1.36	1.27
17	AV	72	Y5P	C2-N3	11.42	1.36	1.27
17	AV	56	Y5P	C2-N3	11.40	1.36	1.27
17	AY	75	Y5P	C2-N3	11.40	1.36	1.27
17	AY	68	Y5P	C2-N3	11.34	1.36	1.27
17	AV	3	Y5P	C2-N3	11.32	1.36	1.27
17	AV	67	Y5P	C2-N3	11.32	1.36	1.27
47	BB	63	Y5P	C2-N3	11.28	1.36	1.27
17	AY	56	Y5P	C2-N3	11.19	1.36	1.27
17	AY	42	Y5P	C2-N3	11.17	1.36	1.27
17	AY	13	Y5P	C2-N3	11.16	1.36	1.27
17	AV	68	Y5P	C2-N3	11.16	1.36	1.27
17	AV	2	Y5P	C2-N3	11.14	1.36	1.27
47	BB	11	Y5P	C2-N3	11.10	1.36	1.27
47	BB	60	Y5P	C2-N3	11.08	1.36	1.27
47	BB	43	Y5P	C2-N3	11.08	1.36	1.27
17	AY	67	Y5P	C2-N3	11.06	1.36	1.27
47	BB	52	Y5P	C2-N3	11.04	1.36	1.27
17	AY	11	Y5P	C2-N3	11.03	1.36	1.27
17	AY	3	Y5P	C2-N3	10.99	1.36	1.27
17	AV	61	Y5P	C2-N3	10.97	1.35	1.27
17	AY	62	Y5P	C2-N3	10.92	1.35	1.27
47	BB	53	Y5P	C2-N3	10.91	1.35	1.27
17	AV	11	Y5P	C2-N3	10.90	1.35	1.27
17	AY	43	Y5P	C2-N3	10.87	1.35	1.27
47	BB	26	Y5P	C2-N3	10.87	1.35	1.27
17	AV	4	Y5P	C2-N3	10.81	1.35	1.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	AV	40	Y5P	C2-N3	10.79	1.35	1.27
17	AV	62	Y5P	C2-N3	10.72	1.35	1.27
47	BB	31	Y5P	C2-N3	10.71	1.35	1.27
47	BB	42	Y5P	C2-N3	10.71	1.35	1.27
17	AY	41	Y5P	C2-N3	10.70	1.35	1.27
17	AY	49	Y5P	C2-N3	10.68	1.35	1.27
18	AX	18	Y5P	C2-N3	10.59	1.35	1.27
17	AY	25	Y5P	C2-N3	10.56	1.35	1.27
17	AY	48	Y5P	C2-N3	10.50	1.35	1.27
17	AV	48	Y5P	C2-N3	10.39	1.35	1.27
17	AY	61	Y5P	C2-N3	10.39	1.35	1.27
17	AV	42	Y5P	C2-N3	10.39	1.35	1.27
47	BB	33	Y5P	C2-N3	10.33	1.35	1.27
18	AX	21	Y5P	C2-N3	10.07	1.35	1.27
17	AV	41	Y5P	C2-N3	10.04	1.35	1.27
17	AY	40	Y5P	C2-N3	9.99	1.35	1.27
17	AV	33	Y5P	C4-N3	-9.63	1.37	1.46
17	AV	75	Y5P	C2-N3	9.40	1.34	1.27
17	AY	33	Y5P	C4-N3	-9.10	1.37	1.46
18	AX	17	Y5P	C4-N3	-8.89	1.37	1.46
17	AY	73	Y5P	C4-N3	-8.88	1.37	1.46
17	AV	24	Y5P	C4-N3	-8.88	1.37	1.46
17	AY	55	Y5P	C4-N3	-8.88	1.37	1.46
17	AY	26	Y5P	C4-N3	-8.86	1.37	1.46
17	AV	52	Y5P	C4-N3	-8.86	1.37	1.46
17	AV	21	Y5P	C4-N3	-8.86	1.37	1.46
17	AY	22	Y5P	C4-N3	-8.86	1.37	1.46
17	AV	64	Y5P	C4-N3	-8.85	1.37	1.46
17	AY	69	Y5P	C4-N3	-8.85	1.37	1.46
17	AY	70	Y5P	C4-N3	-8.85	1.37	1.46
17	AV	73	Y5P	C4-N3	-8.85	1.37	1.46
17	AV	37	Y5P	C4-N3	-8.84	1.38	1.46
17	AV	29	Y5P	C4-N3	-8.83	1.38	1.46
17	AY	9	Y5P	C4-N3	-8.83	1.38	1.46
17	AV	28	Y5P	C4-N3	-8.83	1.38	1.46
17	AY	29	Y5P	C4-N3	-8.83	1.38	1.46
17	AY	44	Y5P	C4-N3	-8.83	1.38	1.46
17	AY	27	Y5P	C4-N3	-8.82	1.38	1.46
17	AY	57	Y5P	C4-N3	-8.82	1.38	1.46
17	AV	5	Y5P	C4-N3	-8.82	1.38	1.46
17	AV	57	Y5P	C4-N3	-8.82	1.38	1.46
17	AY	37	Y5P	C4-N3	-8.82	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	AY	31	Y5P	C4-N3	-8.81	1.38	1.46
17	AV	44	Y5P	C4-N3	-8.81	1.38	1.46
17	AY	63	Y5P	C4-N3	-8.81	1.38	1.46
17	AV	63	Y5P	C4-N3	-8.81	1.38	1.46
17	AY	58	Y5P	C4-N3	-8.81	1.38	1.46
17	AV	14	Y5P	C4-N3	-8.81	1.38	1.46
17	AY	65	Y5P	C4-N3	-8.80	1.38	1.46
17	AY	71	Y5P	C4-N3	-8.80	1.38	1.46
17	AV	27	Y5P	C4-N3	-8.80	1.38	1.46
17	AV	65	Y5P	C4-N3	-8.80	1.38	1.46
17	AV	58	Y5P	C4-N3	-8.80	1.38	1.46
17	AY	38	Y5P	C4-N3	-8.79	1.38	1.46
17	AV	69	Y5P	C4-N3	-8.79	1.38	1.46
17	AV	31	Y5P	C4-N3	-8.79	1.38	1.46
17	AV	30	Y5P	C4-N3	-8.79	1.38	1.46
17	AV	23	Y5P	C4-N3	-8.79	1.38	1.46
17	AV	15	Y5P	C4-N3	-8.79	1.38	1.46
17	AV	71	Y5P	C4-N3	-8.78	1.38	1.46
17	AV	1	Y5P	C4-N3	-8.78	1.38	1.46
17	AY	52	Y5P	C4-N3	-8.78	1.38	1.46
17	AV	26	Y5P	C4-N3	-8.78	1.38	1.46
17	AY	28	Y5P	C4-N3	-8.78	1.38	1.46
17	AY	53	Y5P	C4-N3	-8.78	1.38	1.46
17	AY	24	Y5P	C4-N3	-8.77	1.38	1.46
17	AV	22	Y5P	C4-N3	-8.77	1.38	1.46
17	AV	9	Y5P	C4-N3	-8.77	1.38	1.46
17	AY	6	Y5P	C4-N3	-8.77	1.38	1.46
17	AV	7	Y5P	C4-N3	-8.77	1.38	1.46
17	AY	64	Y5P	C4-N3	-8.76	1.38	1.46
17	AY	1	Y5P	C4-N3	-8.76	1.38	1.46
17	AV	38	Y5P	C4-N3	-8.76	1.38	1.46
17	AV	53	Y5P	C4-N3	-8.76	1.38	1.46
17	AY	7	Y5P	C4-N3	-8.76	1.38	1.46
17	AV	10	Y5P	C4-N3	-8.76	1.38	1.46
17	AV	70	Y5P	C4-N3	-8.75	1.38	1.46
17	AV	6	Y5P	C4-N3	-8.75	1.38	1.46
17	AY	30	Y5P	C4-N3	-8.75	1.38	1.46
17	AY	14	Y5P	C4-N3	-8.75	1.38	1.46
17	AY	5	Y5P	C4-N3	-8.74	1.38	1.46
17	AY	15	Y5P	C4-N3	-8.73	1.38	1.46
17	AY	10	Y5P	C4-N3	-8.72	1.38	1.46
17	AY	23	Y5P	C4-N3	-8.70	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	AY	21	Y5P	C4-N3	-8.69	1.38	1.46
17	AY	45	Y5P	C4-N3	-8.69	1.38	1.46
17	AY	32	Y5P	C4-N3	-8.67	1.38	1.46
47	BB	40	Y5P	C4-N3	-8.60	1.38	1.46
47	BB	44	Y5P	C4-N3	-8.60	1.38	1.46
18	AX	19	Y5P	C4-N3	-8.56	1.38	1.46
17	AV	39	Y5P	C4-N3	-8.52	1.38	1.46
17	AY	50	Y5P	C4-N3	-8.50	1.38	1.46
18	AX	20	Y5P	C4-N3	-8.49	1.38	1.46
47	BB	65	Y5P	C4-N3	-8.43	1.38	1.46
47	BB	6	Y5P	C4-N3	-8.40	1.38	1.46
17	AV	60	Y5P	C4-N3	-8.37	1.38	1.46
17	AV	59	Y5P	C4-N3	-8.37	1.38	1.46
17	AV	8	Y5P	C4-N3	-8.34	1.38	1.46
17	AV	32	Y5P	C4-N3	-8.34	1.38	1.46
18	AX	16	Y5P	C4-N3	-8.34	1.38	1.46
17	AV	55	Y5P	C4-N3	-8.27	1.38	1.46
17	AY	39	Y5P	C4-N3	-8.24	1.38	1.46
17	AY	12	Y5P	C4-N3	-8.21	1.38	1.46
17	AY	59	Y5P	C4-N3	-8.20	1.38	1.46
17	AY	66	Y5P	C4-N3	-8.17	1.38	1.46
17	AV	51	Y5P	C4-N3	-8.14	1.38	1.46
18	AX	13	Y5P	C4-N3	-8.13	1.38	1.46
17	AV	45	Y5P	C4-N3	-8.12	1.38	1.46
17	AY	8	Y5P	C4-N3	-8.09	1.38	1.46
47	BB	8	Y5P	C4-N3	-8.08	1.38	1.46
17	AV	66	Y5P	C4-N3	-8.08	1.38	1.46
17	AV	50	Y5P	C4-N3	-8.07	1.38	1.46
17	AY	60	Y5P	C4-N3	-8.07	1.38	1.46
47	BB	34	Y5P	C4-N3	-8.06	1.38	1.46
47	BB	48	Y5P	C4-N3	-8.03	1.38	1.46
47	BB	62	Y5P	C4-N3	-8.00	1.38	1.46
18	AX	14	Y5P	C4-N3	-7.96	1.38	1.46
17	AV	54	Y5P	C4-N3	-7.95	1.38	1.46
17	AY	54	Y5P	C4-N3	-7.94	1.38	1.46
17	AY	51	Y5P	C4-N3	-7.91	1.38	1.46
18	AX	24	Y5P	C4-N3	-7.91	1.38	1.46
47	BB	13	Y5P	C4-N3	-7.91	1.38	1.46
47	BB	61	Y5P	C4-N3	-7.90	1.38	1.46
47	BB	12	Y5P	C4-N3	-7.87	1.38	1.46
18	AX	22	Y5P	C4-N3	-7.85	1.38	1.46
18	AX	12	Y5P	C4-N3	-7.84	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	AV	12	Y5P	C4-N3	-7.67	1.39	1.46
18	AX	23	Y5P	C4-N3	-7.66	1.39	1.46
18	AX	15	Y5P	C4-N3	-7.45	1.39	1.46
17	AY	73	Y5P	C1'-N1	5.00	1.60	1.46
17	AV	21	Y5P	C1'-N1	4.98	1.60	1.46
17	AV	57	Y5P	C1'-N1	4.93	1.59	1.46
17	AV	27	Y5P	C1'-N1	4.87	1.59	1.46
17	AV	14	Y5P	C1'-N1	4.78	1.59	1.46
17	AV	70	Y5P	C1'-N1	4.72	1.59	1.46
17	AY	26	Y5P	C1'-N1	4.71	1.59	1.46
17	AY	64	Y5P	C1'-N1	4.71	1.59	1.46
17	AV	73	Y5P	C1'-N1	4.68	1.59	1.46
17	AV	64	Y5P	C1'-N1	4.67	1.59	1.46
17	AV	44	Y5P	C1'-N1	4.64	1.59	1.46
17	AY	70	Y5P	C1'-N1	4.62	1.59	1.46
17	AY	21	Y5P	C1'-N1	4.60	1.59	1.46
17	AY	65	Y5P	C1'-N1	4.56	1.58	1.46
17	AV	5	Y5P	C1'-N1	4.54	1.58	1.46
17	AY	71	Y5P	C1'-N1	4.52	1.58	1.46
17	AY	44	Y5P	C1'-N1	4.52	1.58	1.46
17	AY	23	Y5P	C1'-N1	4.47	1.58	1.46
17	AY	1	Y5P	C1'-N1	4.46	1.58	1.46
17	AV	26	Y5P	C1'-N1	4.45	1.58	1.46
17	AV	58	Y5P	C1'-N1	4.40	1.58	1.46
17	AV	30	Y5P	C1'-N1	4.39	1.58	1.46
17	AY	37	Y5P	C1'-N1	4.38	1.58	1.46
17	AY	31	Y5P	C1'-N1	4.37	1.58	1.46
17	AY	15	Y5P	C1'-N1	4.37	1.58	1.46
17	AV	31	Y5P	C1'-N1	4.37	1.58	1.46
17	AY	27	Y5P	C1'-N1	4.36	1.58	1.46
17	AV	69	Y5P	C1'-N1	4.35	1.58	1.46
17	AV	22	Y5P	C1'-N1	4.34	1.58	1.46
17	AV	37	Y5P	C1'-N1	4.34	1.58	1.46
17	AY	28	Y5P	C1'-N1	4.30	1.58	1.46
17	AV	65	Y5P	C1'-N1	4.28	1.58	1.46
17	AY	38	Y5P	C1'-N1	4.25	1.58	1.46
17	AY	57	Y5P	C1'-N1	4.22	1.58	1.46
17	AY	30	Y5P	C1'-N1	4.22	1.58	1.46
17	AY	24	Y5P	C1'-N1	4.20	1.57	1.46
17	AY	14	Y5P	C1'-N1	4.20	1.57	1.46
17	AV	6	Y5P	C1'-N1	4.19	1.57	1.46
17	AY	69	Y5P	C1'-N1	4.16	1.57	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	AV	53	Y5P	C1'-N1	4.15	1.57	1.46
17	AY	6	Y5P	C1'-N1	4.15	1.57	1.46
17	AY	7	Y5P	C1'-N1	4.13	1.57	1.46
17	AY	53	Y5P	C1'-N1	4.12	1.57	1.46
17	AY	63	Y5P	C1'-N1	4.11	1.57	1.46
17	AY	5	Y5P	C1'-N1	4.11	1.57	1.46
17	AY	58	Y5P	C1'-N1	4.10	1.57	1.46
17	AY	10	Y5P	C1'-N1	4.09	1.57	1.46
17	AV	15	Y5P	C1'-N1	4.08	1.57	1.46
17	AV	71	Y5P	C1'-N1	4.08	1.57	1.46
17	AV	10	Y5P	C1'-N1	4.06	1.57	1.46
17	AV	28	Y5P	C1'-N1	4.06	1.57	1.46
17	AV	24	Y5P	C1'-N1	4.06	1.57	1.46
17	AV	38	Y5P	C1'-N1	4.03	1.57	1.46
17	AV	63	Y5P	C1'-N1	4.02	1.57	1.46
17	AV	9	Y5P	C1'-N1	4.01	1.57	1.46
17	AV	23	Y5P	C1'-N1	3.99	1.57	1.46
17	AV	52	Y5P	C1'-N1	3.96	1.57	1.46
17	AY	9	Y5P	C1'-N1	3.89	1.57	1.46
17	AY	29	Y5P	C1'-N1	3.89	1.57	1.46
17	AY	22	Y5P	C1'-N1	3.88	1.57	1.46
17	AY	52	Y5P	C1'-N1	3.86	1.56	1.46
17	AV	1	Y5P	C1'-N1	3.83	1.56	1.46
17	AV	7	Y5P	C1'-N1	3.57	1.56	1.46
17	AV	34	P5P	C6-N1	3.04	1.40	1.34
17	AV	29	Y5P	C1'-N1	3.01	1.54	1.46
47	BB	35	P5P	C6-N1	2.77	1.40	1.34
47	BB	49	P5P	C6-N1	2.75	1.40	1.34
47	BB	25	P5P	C6-N1	2.69	1.40	1.34
17	AV	34	P5P	C6-C5	2.66	1.43	1.39
47	BB	41	P5P	C6-N1	2.65	1.39	1.34
17	AY	34	P5P	C6-N1	2.65	1.39	1.34
47	BB	51	P5P	C6-N1	2.59	1.39	1.34
47	BB	59	P5P	C6-N1	2.57	1.39	1.34
47	BB	29	P5P	C6-N1	2.56	1.39	1.34
47	BB	35	P5P	C6-C5	2.55	1.43	1.39
17	AV	34	P5P	C2-N1	2.51	1.38	1.33
47	BB	7	P5P	C6-N1	2.50	1.39	1.34
17	AY	34	P5P	C2-N1	2.50	1.38	1.33
47	BB	30	P5P	C6-N1	2.48	1.39	1.34
47	BB	30	P5P	C6-C5	2.47	1.43	1.39
47	BB	49	P5P	C2-N1	2.37	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	BB	10	P5P	C6-N1	2.37	1.39	1.34
47	BB	46	P5P	C6-N1	2.33	1.39	1.34
47	BB	25	P5P	C2-N1	2.32	1.38	1.33
47	BB	49	P5P	C6-C5	2.29	1.42	1.39
47	BB	51	P5P	C2-N1	2.27	1.37	1.33
47	BB	59	P5P	C2-N1	2.27	1.37	1.33
47	BB	35	P5P	C2-N1	2.25	1.37	1.33
47	BB	7	P5P	C2-N1	2.20	1.37	1.33
47	BB	41	P5P	C2-N1	2.19	1.37	1.33
47	BB	10	P5P	C2-N1	2.18	1.37	1.33
47	BB	29	P5P	C2-N1	2.18	1.37	1.33
47	BB	59	P5P	C6-C5	2.15	1.42	1.39
47	BB	25	P5P	C6-C5	2.05	1.42	1.39
47	BB	46	P5P	C2-N1	2.04	1.37	1.33
17	AY	76	P5P	C6-C5	2.03	1.42	1.39
47	BB	7	P5P	C6-C5	2.02	1.42	1.39
47	BB	46	P5P	C6-C5	2.01	1.42	1.39

All (290) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	AV	34	P5P	C6-N1-C2	8.50	125.83	115.80
47	BB	7	P5P	C6-N1-C2	8.24	125.52	115.80
47	BB	41	P5P	C6-N1-C2	8.16	125.43	115.80
17	AY	34	P5P	C6-N1-C2	8.14	125.41	115.80
47	BB	49	P5P	C6-N1-C2	7.97	125.20	115.80
47	BB	51	P5P	C6-N1-C2	7.90	125.13	115.80
47	BB	29	P5P	C6-N1-C2	7.87	125.09	115.80
47	BB	35	P5P	C6-N1-C2	7.87	125.08	115.80
47	BB	59	P5P	C6-N1-C2	7.76	124.96	115.80
47	BB	10	P5P	C6-N1-C2	7.65	124.83	115.80
47	BB	46	P5P	C6-N1-C2	7.59	124.75	115.80
47	BB	25	P5P	C6-N1-C2	7.43	124.57	115.80
47	BB	30	P5P	C6-N1-C2	7.25	124.36	115.80
47	BB	42	Y5P	C5-C4-N3	5.08	122.35	114.15
17	AV	75	Y5P	C5-C4-N3	5.07	122.32	114.15
17	AV	48	Y5P	C5-C4-N3	5.02	122.25	114.15
17	AY	40	Y5P	C5-C4-N3	4.99	122.20	114.15
17	AY	61	Y5P	C5-C4-N3	4.99	122.19	114.15
17	AV	41	Y5P	C5-C4-N3	4.96	122.14	114.15
17	AV	11	Y5P	C5-C4-N3	4.96	122.14	114.15
17	AY	41	Y5P	C5-C4-N3	4.94	122.12	114.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	AY	42	Y5P	C5-C4-N3	4.93	122.09	114.15
17	AY	49	Y5P	C5-C4-N3	4.91	122.06	114.15
18	AX	21	Y5P	C5-C4-N3	4.90	122.05	114.15
17	AY	3	Y5P	C5-C4-N3	4.84	121.95	114.15
17	AV	62	Y5P	C5-C4-N3	4.82	121.93	114.15
47	BB	43	Y5P	C5-C4-N3	4.78	121.85	114.15
17	AY	13	Y5P	C5-C4-N3	4.77	121.85	114.15
47	BB	33	Y5P	C5-C4-N3	4.77	121.84	114.15
17	AY	62	Y5P	C5-C4-N3	4.77	121.84	114.15
47	BB	53	Y5P	C5-C4-N3	4.75	121.81	114.15
47	BB	31	Y5P	C5-C4-N3	4.74	121.80	114.15
17	AY	48	Y5P	C5-C4-N3	4.74	121.80	114.15
17	AY	43	Y5P	C5-C4-N3	4.72	121.77	114.15
17	AY	11	Y5P	C5-C4-N3	4.71	121.75	114.15
17	AY	56	Y5P	C5-C4-N3	4.69	121.71	114.15
47	BB	26	Y5P	C5-C4-N3	4.67	121.68	114.15
47	BB	60	Y5P	C5-C4-N3	4.66	121.67	114.15
17	AY	25	Y5P	C5-C4-N3	4.66	121.66	114.15
47	BB	52	Y5P	C5-C4-N3	4.65	121.64	114.15
17	AY	75	Y5P	C5-C4-N3	4.63	121.61	114.15
17	AV	61	Y5P	C5-C4-N3	4.61	121.59	114.15
47	BB	11	Y5P	C5-C4-N3	4.61	121.59	114.15
17	AY	4	Y5P	C5-C4-N3	4.59	121.55	114.15
17	AV	68	Y5P	C5-C4-N3	4.58	121.54	114.15
17	AY	67	Y5P	C5-C4-N3	4.58	121.53	114.15
17	AV	72	Y5P	C5-C4-N3	4.57	121.53	114.15
17	AV	40	Y5P	C5-C4-N3	4.57	121.51	114.15
18	AX	18	Y5P	C5-C4-N3	4.56	121.50	114.15
17	AV	49	Y5P	C5-C4-N3	4.56	121.50	114.15
17	AV	13	Y5P	C5-C4-N3	4.55	121.49	114.15
17	AV	56	Y5P	C5-C4-N3	4.54	121.46	114.15
17	AV	4	Y5P	C5-C4-N3	4.52	121.44	114.15
17	AV	42	Y5P	C5-C4-N3	4.51	121.43	114.15
17	AY	68	Y5P	C5-C4-N3	4.49	121.39	114.15
17	AV	67	Y5P	C5-C4-N3	4.42	121.28	114.15
17	AY	74	Y5P	C5-C4-N3	4.41	121.26	114.15
17	AV	3	Y5P	C5-C4-N3	4.38	121.22	114.15
17	AY	34	P5P	C5-C6-N1	-4.38	111.00	121.90
17	AV	25	Y5P	C5-C4-N3	4.37	121.19	114.15
17	AV	34	P5P	C5-C6-N1	-4.32	111.14	121.90
47	BB	63	Y5P	C5-C4-N3	4.30	121.09	114.15
47	BB	7	P5P	C5-C6-N1	-4.30	111.19	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	AV	43	Y5P	C5-C4-N3	4.27	121.03	114.15
17	AY	72	Y5P	C5-C4-N3	4.23	120.97	114.15
17	AY	2	Y5P	C5-C4-N3	4.22	120.96	114.15
47	BB	10	P5P	C5-C6-N1	-4.17	111.51	121.90
47	BB	49	P5P	C5-C6-N1	-4.12	111.64	121.90
47	BB	46	P5P	C5-C6-N1	-4.12	111.65	121.90
47	BB	51	P5P	C5-C6-N1	-4.08	111.75	121.90
47	BB	41	P5P	C5-C6-N1	-4.06	111.80	121.90
17	AV	8	Y5P	N1-C2-N3	-4.04	114.18	125.39
17	AV	2	Y5P	C5-C4-N3	4.02	120.63	114.15
47	BB	59	P5P	C5-C6-N1	-4.01	111.91	121.90
47	BB	13	Y5P	N1-C2-N3	-4.00	114.28	125.39
17	AY	51	Y5P	N1-C2-N3	-3.98	114.35	125.39
17	AY	54	Y5P	N1-C2-N3	-3.98	114.36	125.39
47	BB	8	Y5P	N1-C2-N3	-3.97	114.38	125.39
47	BB	35	P5P	C5-C6-N1	-3.92	112.13	121.90
17	AV	74	Y5P	C5-C4-N3	3.92	120.47	114.15
17	AV	12	Y5P	N1-C2-N3	-3.90	114.57	125.39
47	BB	25	P5P	C5-C6-N1	-3.90	112.18	121.90
17	AY	39	Y5P	N1-C2-N3	-3.87	114.65	125.39
18	AX	23	Y5P	N1-C2-N3	-3.87	114.66	125.39
47	BB	29	P5P	C5-C6-N1	-3.84	112.33	121.90
18	AX	12	Y5P	N1-C2-N3	-3.84	114.75	125.39
17	AY	8	Y5P	N1-C2-N3	-3.83	114.76	125.39
18	AX	15	Y5P	N1-C2-N3	-3.82	114.79	125.39
17	AV	54	Y5P	N1-C2-N3	-3.81	114.84	125.39
18	AX	16	Y5P	N1-C2-N3	-3.80	114.85	125.39
47	BB	62	Y5P	N1-C2-N3	-3.80	114.86	125.39
47	BB	48	Y5P	N1-C2-N3	-3.80	114.86	125.39
18	AX	13	Y5P	N1-C2-N3	-3.80	114.87	125.39
17	AY	50	Y5P	N1-C2-N3	-3.79	114.88	125.39
17	AV	39	Y5P	N1-C2-N3	-3.78	114.90	125.39
17	AY	45	Y5P	N1-C2-N3	-3.78	114.91	125.39
47	BB	65	Y5P	N1-C2-N3	-3.77	114.95	125.39
17	AY	12	Y5P	N1-C2-N3	-3.76	114.97	125.39
17	AV	32	Y5P	N1-C2-N3	-3.74	115.01	125.39
17	AV	59	Y5P	N1-C2-N3	-3.73	115.04	125.39
18	AX	17	Y5P	N1-C2-N3	-3.73	115.04	125.39
18	AX	22	Y5P	N1-C2-N3	-3.71	115.09	125.39
47	BB	30	P5P	C5-C6-N1	-3.71	112.65	121.90
17	AY	66	Y5P	N1-C2-N3	-3.71	115.11	125.39
17	AY	59	Y5P	N1-C2-N3	-3.71	115.11	125.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	AX	20	Y5P	N1-C2-N3	-3.70	115.14	125.39
17	AV	52	Y5P	N1-C2-N3	-3.69	115.17	125.39
17	AY	60	Y5P	N1-C2-N3	-3.69	115.17	125.39
17	AY	6	Y5P	N1-C2-N3	-3.68	115.18	125.39
17	AV	73	Y5P	N1-C2-N3	-3.68	115.18	125.39
17	AV	70	Y5P	N1-C2-N3	-3.68	115.18	125.39
17	AY	15	Y5P	N1-C2-N3	-3.68	115.18	125.39
17	AY	22	Y5P	N1-C2-N3	-3.68	115.19	125.39
17	AV	9	Y5P	N1-C2-N3	-3.68	115.19	125.39
17	AY	64	Y5P	N1-C2-N3	-3.68	115.19	125.39
17	AV	27	Y5P	N1-C2-N3	-3.68	115.19	125.39
17	AV	53	Y5P	N1-C2-N3	-3.68	115.19	125.39
17	AV	14	Y5P	N1-C2-N3	-3.68	115.19	125.39
17	AV	69	Y5P	N1-C2-N3	-3.68	115.19	125.39
17	AV	71	Y5P	N1-C2-N3	-3.68	115.19	125.39
17	AY	44	Y5P	N1-C2-N3	-3.68	115.19	125.39
17	AV	64	Y5P	N1-C2-N3	-3.68	115.19	125.39
17	AV	6	Y5P	N1-C2-N3	-3.68	115.20	125.39
17	AV	23	Y5P	N1-C2-N3	-3.67	115.20	125.39
17	AY	65	Y5P	N1-C2-N3	-3.67	115.21	125.39
17	AY	30	Y5P	N1-C2-N3	-3.67	115.21	125.39
17	AY	31	Y5P	N1-C2-N3	-3.67	115.21	125.39
17	AV	57	Y5P	N1-C2-N3	-3.67	115.21	125.39
17	AY	37	Y5P	N1-C2-N3	-3.67	115.21	125.39
17	AV	26	Y5P	N1-C2-N3	-3.67	115.21	125.39
17	AY	71	Y5P	N1-C2-N3	-3.67	115.21	125.39
17	AV	24	Y5P	N1-C2-N3	-3.67	115.21	125.39
17	AY	53	Y5P	N1-C2-N3	-3.67	115.22	125.39
17	AY	57	Y5P	N1-C2-N3	-3.67	115.22	125.39
17	AV	44	Y5P	N1-C2-N3	-3.67	115.22	125.39
17	AY	29	Y5P	N1-C2-N3	-3.67	115.22	125.39
17	AY	28	Y5P	N1-C2-N3	-3.67	115.22	125.39
17	AY	70	Y5P	N1-C2-N3	-3.67	115.22	125.39
17	AV	37	Y5P	N1-C2-N3	-3.67	115.22	125.39
17	AY	1	Y5P	N1-C2-N3	-3.67	115.22	125.39
17	AY	7	Y5P	N1-C2-N3	-3.67	115.22	125.39
17	AV	63	Y5P	N1-C2-N3	-3.67	115.22	125.39
17	AY	73	Y5P	N1-C2-N3	-3.67	115.22	125.39
17	AV	1	Y5P	N1-C2-N3	-3.67	115.22	125.39
17	AV	30	Y5P	N1-C2-N3	-3.67	115.22	125.39
17	AY	23	Y5P	N1-C2-N3	-3.66	115.23	125.39
17	AY	26	Y5P	N1-C2-N3	-3.66	115.23	125.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	AV	29	Y5P	N1-C2-N3	-3.66	115.23	125.39
17	AV	7	Y5P	N1-C2-N3	-3.66	115.23	125.39
17	AV	31	Y5P	N1-C2-N3	-3.66	115.23	125.39
17	AV	22	Y5P	N1-C2-N3	-3.66	115.24	125.39
17	AY	63	Y5P	N1-C2-N3	-3.66	115.24	125.39
17	AV	5	Y5P	N1-C2-N3	-3.66	115.24	125.39
17	AY	58	Y5P	N1-C2-N3	-3.66	115.24	125.39
17	AY	69	Y5P	N1-C2-N3	-3.66	115.24	125.39
17	AY	5	Y5P	N1-C2-N3	-3.66	115.25	125.39
17	AY	38	Y5P	N1-C2-N3	-3.66	115.25	125.39
17	AV	65	Y5P	N1-C2-N3	-3.66	115.25	125.39
17	AY	21	Y5P	N1-C2-N3	-3.66	115.25	125.39
17	AY	27	Y5P	N1-C2-N3	-3.66	115.25	125.39
17	AY	52	Y5P	N1-C2-N3	-3.66	115.25	125.39
17	AV	28	Y5P	N1-C2-N3	-3.65	115.25	125.39
17	AV	10	Y5P	N1-C2-N3	-3.65	115.26	125.39
17	AY	10	Y5P	N1-C2-N3	-3.65	115.26	125.39
17	AV	21	Y5P	N1-C2-N3	-3.65	115.26	125.39
17	AV	15	Y5P	N1-C2-N3	-3.65	115.27	125.39
17	AV	38	Y5P	N1-C2-N3	-3.65	115.27	125.39
17	AV	58	Y5P	N1-C2-N3	-3.65	115.27	125.39
17	AY	14	Y5P	N1-C2-N3	-3.65	115.27	125.39
17	AY	9	Y5P	N1-C2-N3	-3.65	115.27	125.39
17	AY	24	Y5P	N1-C2-N3	-3.65	115.27	125.39
47	BB	12	Y5P	N1-C2-N3	-3.61	115.38	125.39
17	AY	32	Y5P	N1-C2-N3	-3.59	115.42	125.39
17	AV	60	Y5P	N1-C2-N3	-3.59	115.43	125.39
18	AX	19	Y5P	N1-C2-N3	-3.59	115.43	125.39
17	AV	50	Y5P	N1-C2-N3	-3.58	115.47	125.39
47	BB	6	Y5P	N1-C2-N3	-3.56	115.52	125.39
47	BB	61	Y5P	N1-C2-N3	-3.56	115.53	125.39
47	BB	40	Y5P	N1-C2-N3	-3.53	115.60	125.39
17	AY	55	Y5P	N1-C2-N3	-3.52	115.61	125.39
17	AY	73	Y5P	C1'-N1-C6	-3.51	113.35	120.77
17	AV	66	Y5P	N1-C2-N3	-3.48	115.73	125.39
18	AX	24	Y5P	N1-C2-N3	-3.46	115.80	125.39
17	AV	51	Y5P	N1-C2-N3	-3.44	115.85	125.39
18	AX	14	Y5P	N1-C2-N3	-3.43	115.89	125.39
47	BB	34	Y5P	N1-C2-N3	-3.42	115.90	125.39
17	AV	55	Y5P	N1-C2-N3	-3.42	115.91	125.39
47	BB	44	Y5P	N1-C2-N3	-3.37	116.05	125.39
17	AY	33	Y5P	N1-C2-N3	-3.29	116.25	125.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	AV	45	Y5P	N1-C2-N3	-3.29	116.26	125.39
47	BB	23	P5P	C6-N1-C2	3.17	119.54	115.80
47	BB	10	P5P	C6-C5-C4	3.07	119.59	116.24
17	AV	33	Y5P	N1-C2-N3	-2.96	117.19	125.39
47	BB	23	P5P	C4-N9-C1'	-2.92	119.80	126.63
47	BB	23	P5P	C1'-N9-C8	2.90	133.53	127.09
17	AY	34	P5P	C6-C5-C4	2.84	119.34	116.24
17	AY	69	Y5P	C1'-N1-C6	-2.81	114.83	120.77
17	AY	27	Y5P	C1'-N1-C6	-2.80	114.86	120.77
47	BB	47	P5P	C6-N1-C2	2.79	119.09	115.80
17	AV	76	P5P	C6-N1-C2	2.61	118.88	115.80
47	BB	25	P5P	C6-C5-C4	2.60	119.09	116.24
47	BB	46	P5P	C6-C5-C4	2.60	119.09	116.24
17	AV	36	P5P	C6-N1-C2	2.60	118.87	115.80
17	AV	35	P5P	C6-N1-C2	2.59	118.86	115.80
47	BB	23	P5P	O4'-C1'-N9	2.56	113.01	108.09
17	AV	73	Y5P	C1'-N1-C6	-2.54	115.40	120.77
47	BB	59	P5P	C6-C5-C4	2.52	118.99	116.24
47	BB	51	P5P	C6-C5-C4	2.51	118.99	116.24
17	AY	73	Y5P	O4'-C1'-N1	2.51	112.87	108.08
47	BB	41	P5P	C6-C5-C4	2.48	118.95	116.24
47	BB	39	P5P	C6-N1-C2	2.48	118.73	115.80
17	AY	76	P5P	C6-N1-C2	2.47	118.71	115.80
47	BB	41	P5P	N1-C2-N3	-2.46	123.14	127.33
47	BB	7	P5P	C6-C5-C4	2.42	118.89	116.24
47	BB	36	P5P	C6-N1-C2	2.41	118.65	115.80
17	AY	62	Y5P	N1-C2-N3	-2.41	118.70	125.39
47	BB	26	Y5P	N1-C2-N3	-2.41	118.70	125.39
47	BB	29	P5P	N1-C2-N3	-2.41	123.23	127.33
47	BB	38	P5P	C6-N1-C2	2.41	118.64	115.80
17	AY	3	Y5P	N1-C2-N3	-2.41	118.71	125.39
47	BB	66	P5P	C6-N1-C2	2.40	118.64	115.80
17	AY	42	Y5P	N1-C2-N3	-2.40	118.72	125.39
17	AV	11	Y5P	N1-C2-N3	-2.40	118.75	125.39
17	AV	62	Y5P	N1-C2-N3	-2.38	118.78	125.39
17	AY	40	Y5P	N1-C2-N3	-2.38	118.80	125.39
47	BB	5	P5P	C6-N1-C2	2.38	118.61	115.80
17	AY	43	Y5P	N1-C2-N3	-2.37	118.82	125.39
17	AY	13	Y5P	N1-C2-N3	-2.37	118.83	125.39
17	AY	35	P5P	C6-N1-C2	2.36	118.59	115.80
17	AY	36	P5P	C6-N1-C2	2.36	118.58	115.80
47	BB	60	Y5P	N1-C2-N3	-2.35	118.86	125.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	AY	4	Y5P	N1-C2-N3	-2.35	118.87	125.39
47	BB	35	P5P	N1-C2-N3	-2.35	123.34	127.33
47	BB	37	P5P	C6-N1-C2	2.34	118.57	115.80
17	AY	41	Y5P	N1-C2-N3	-2.33	118.92	125.39
17	AV	13	Y5P	N1-C2-N3	-2.32	118.94	125.39
47	BB	30	P5P	C6-C5-C4	2.32	118.78	116.24
17	AV	1	Y5P	C1'-N1-C6	-2.32	115.86	120.77
17	AY	61	Y5P	N1-C2-N3	-2.32	118.97	125.39
17	AY	25	Y5P	N1-C2-N3	-2.31	118.97	125.39
17	AV	34	P5P	N1-C2-N3	-2.31	123.40	127.33
47	BB	33	Y5P	N1-C2-N3	-2.30	119.00	125.39
17	AY	49	Y5P	N1-C2-N3	-2.30	119.02	125.39
17	AY	68	Y5P	N1-C2-N3	-2.28	119.07	125.39
47	BB	14	P5P	C6-N1-C2	2.28	118.49	115.80
17	AY	2	Y5P	N1-C2-N3	-2.28	119.08	125.39
47	BB	58	P5P	C6-N1-C2	2.27	118.48	115.80
47	BB	9	P5P	C6-N1-C2	2.27	118.48	115.80
47	BB	52	Y5P	N1-C2-N3	-2.27	119.11	125.39
47	BB	31	Y5P	N1-C2-N3	-2.26	119.12	125.39
47	BB	53	Y5P	N1-C2-N3	-2.24	119.17	125.39
47	BB	43	Y5P	N1-C2-N3	-2.23	119.19	125.39
17	AY	56	Y5P	N1-C2-N3	-2.22	119.22	125.39
17	AV	49	Y5P	N1-C2-N3	-2.21	119.25	125.39
47	BB	63	Y5P	N1-C2-N3	-2.20	119.30	125.39
47	BB	15	P5P	C6-N1-C2	2.20	118.39	115.80
17	AY	75	Y5P	N1-C2-N3	-2.19	119.32	125.39
47	BB	42	Y5P	N1-C2-N3	-2.18	119.33	125.39
17	AV	75	Y5P	N1-C2-N3	-2.18	119.34	125.39
17	AY	55	Y5P	C1'-N1-C6	-2.17	116.19	120.77
17	AY	48	Y5P	N1-C2-N3	-2.17	119.38	125.39
17	AV	48	Y5P	N1-C2-N3	-2.15	119.42	125.39
17	AY	15	Y5P	C1'-N1-C6	-2.15	116.23	120.77
17	AV	56	Y5P	N1-C2-N3	-2.15	119.43	125.39
17	AV	4	Y5P	N1-C2-N3	-2.14	119.44	125.39
47	BB	51	P5P	N1-C2-N3	-2.13	123.71	127.33
47	BB	30	P5P	N1-C2-N3	-2.13	123.71	127.33
17	AY	11	Y5P	N1-C2-N3	-2.12	119.51	125.39
17	AV	61	Y5P	N1-C2-N3	-2.12	119.51	125.39
47	BB	59	P5P	N1-C2-N3	-2.11	123.74	127.33
47	BB	49	P5P	N1-C2-N3	-2.11	123.75	127.33
17	AV	68	Y5P	N1-C2-N3	-2.10	119.57	125.39
17	AV	40	Y5P	N1-C2-N3	-2.09	119.59	125.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	AV	41	Y5P	N1-C2-N3	-2.09	119.59	125.39
17	AV	27	Y5P	C1'-N1-C6	-2.09	116.36	120.77
47	BB	25	P5P	N1-C2-N3	-2.08	123.79	127.33
17	AV	42	Y5P	N1-C2-N3	-2.07	119.64	125.39
17	AV	73	Y5P	O4'-C1'-N1	2.07	112.03	108.08
17	AY	74	Y5P	N1-C2-N3	-2.06	119.67	125.39
18	AX	18	Y5P	N1-C2-N3	-2.06	119.67	125.39
47	BB	64	P5P	C6-N1-C2	2.06	118.23	115.80
17	AV	43	Y5P	N1-C2-N3	-2.05	119.71	125.39
17	AV	67	Y5P	N1-C2-N3	-2.05	119.71	125.39
17	AV	34	P5P	C6-C5-C4	2.04	118.47	116.24
47	BB	49	P5P	C6-C5-C4	2.04	118.47	116.24
17	AV	74	Y5P	N1-C2-N3	-2.04	119.74	125.39
47	BB	47	P5P	C5-C6-N1	-2.03	116.84	121.90
47	BB	28	P5P	C6-N1-C2	2.01	118.18	115.80
17	AV	3	Y5P	N1-C2-N3	-2.00	119.83	125.39
18	AX	21	Y5P	N1-C2-N3	-2.00	119.84	125.39

There are no chirality outliers.

All (296) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	AV	76	P5P	C4'-C5'-O5'-P
17	AY	34	P5P	O4'-C4'-C5'-O5'
47	BB	5	P5P	O4'-C4'-C5'-O5'
47	BB	15	P5P	O4'-C4'-C5'-O5'
47	BB	23	P5P	C4'-C5'-O5'-P
47	BB	35	P5P	O4'-C4'-C5'-O5'
17	AY	2	Y5P	O4'-C1'-N1-C2
17	AV	3	Y5P	O4'-C1'-N1-C2
17	AY	3	Y5P	O4'-C1'-N1-C2
17	AY	5	Y5P	O4'-C1'-N1-C2
17	AV	6	Y5P	O4'-C4'-C5'-O5'
17	AY	6	Y5P	O4'-C1'-N1-C2
17	AY	8	Y5P	O4'-C1'-N1-C2
17	AV	9	Y5P	C2'-C1'-N1-C6
17	AY	11	Y5P	O4'-C1'-N1-C2
17	AY	13	Y5P	O4'-C1'-N1-C2
17	AV	14	Y5P	O4'-C1'-N1-C2
17	AY	15	Y5P	O4'-C4'-C5'-O5'
17	AV	22	Y5P	O4'-C4'-C5'-O5'
17	AV	22	Y5P	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
17	AV	25	Y5P	O4'-C1'-N1-C2
17	AY	25	Y5P	O4'-C1'-N1-C2
17	AV	27	Y5P	O4'-C1'-N1-C2
17	AY	30	Y5P	O4'-C4'-C5'-O5'
17	AV	32	Y5P	O4'-C4'-C5'-O5'
17	AV	32	Y5P	O4'-C1'-N1-C2
17	AY	32	Y5P	O4'-C1'-N1-C2
17	AV	33	Y5P	O4'-C1'-N1-C2
17	AV	42	Y5P	O4'-C4'-C5'-O5'
17	AV	42	Y5P	C3'-C4'-C5'-O5'
17	AV	42	Y5P	O4'-C1'-N1-C2
17	AY	43	Y5P	C4'-C5'-O5'-P
17	AY	43	Y5P	O4'-C1'-N1-C2
17	AV	48	Y5P	O4'-C4'-C5'-O5'
17	AV	48	Y5P	C3'-C4'-C5'-O5'
17	AY	48	Y5P	O4'-C1'-N1-C2
17	AY	49	Y5P	O4'-C1'-N1-C2
17	AV	53	Y5P	O4'-C1'-N1-C2
17	AY	54	Y5P	O4'-C1'-N1-C2
17	AV	56	Y5P	O4'-C1'-N1-C2
17	AV	58	Y5P	C2'-C1'-N1-C6
17	AV	59	Y5P	O4'-C4'-C5'-O5'
17	AV	61	Y5P	O4'-C1'-N1-C2
17	AY	61	Y5P	O4'-C1'-N1-C2
17	AV	62	Y5P	O4'-C1'-N1-C2
17	AY	64	Y5P	O4'-C1'-N1-C2
17	AV	66	Y5P	O4'-C1'-N1-C2
17	AY	66	Y5P	O4'-C1'-N1-C2
17	AY	74	Y5P	C4'-C5'-O5'-P
17	AY	74	Y5P	O4'-C1'-N1-C2
17	AV	75	Y5P	O4'-C4'-C5'-O5'
18	AX	12	Y5P	O4'-C1'-N1-C2
18	AX	13	Y5P	O4'-C1'-N1-C2
18	AX	14	Y5P	O4'-C1'-N1-C2
18	AX	23	Y5P	O4'-C4'-C5'-O5'
18	AX	23	Y5P	O4'-C1'-N1-C2
18	AX	24	Y5P	O4'-C1'-N1-C2
47	BB	6	Y5P	O4'-C1'-N1-C2
47	BB	42	Y5P	O4'-C1'-N1-C2
47	BB	44	Y5P	O4'-C4'-C5'-O5'
47	BB	52	Y5P	O4'-C1'-N1-C2
47	BB	61	Y5P	O4'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
47	BB	63	Y5P	O4'-C1'-N1-C2
17	AV	1	Y5P	O4'-C1'-N1-C2
17	AY	1	Y5P	O4'-C1'-N1-C2
17	AV	2	Y5P	O4'-C1'-N1-C2
17	AV	4	Y5P	O4'-C1'-N1-C2
17	AY	4	Y5P	O4'-C1'-N1-C2
17	AV	5	Y5P	O4'-C1'-N1-C2
17	AV	6	Y5P	O4'-C1'-N1-C2
17	AV	7	Y5P	O4'-C1'-N1-C2
17	AV	8	Y5P	O4'-C1'-N1-C2
17	AY	9	Y5P	O4'-C1'-N1-C2
17	AV	10	Y5P	O4'-C1'-N1-C2
17	AY	10	Y5P	O4'-C1'-N1-C2
17	AV	11	Y5P	O4'-C1'-N1-C2
17	AV	12	Y5P	O4'-C1'-N1-C2
17	AY	12	Y5P	O4'-C1'-N1-C2
17	AV	13	Y5P	O4'-C1'-N1-C2
17	AY	14	Y5P	O4'-C1'-N1-C2
17	AV	15	Y5P	O4'-C1'-N1-C2
17	AY	15	Y5P	O4'-C1'-N1-C2
17	AV	21	Y5P	O4'-C1'-N1-C2
17	AY	21	Y5P	O4'-C1'-N1-C2
17	AV	22	Y5P	O4'-C1'-N1-C2
17	AY	22	Y5P	O4'-C1'-N1-C2
17	AV	23	Y5P	O4'-C1'-N1-C2
17	AY	23	Y5P	O4'-C1'-N1-C2
17	AV	24	Y5P	O4'-C1'-N1-C2
17	AY	24	Y5P	O4'-C1'-N1-C2
17	AV	26	Y5P	O4'-C1'-N1-C2
17	AY	26	Y5P	O4'-C1'-N1-C2
17	AY	27	Y5P	O4'-C1'-N1-C2
17	AV	28	Y5P	O4'-C1'-N1-C2
17	AY	28	Y5P	O4'-C1'-N1-C2
17	AV	29	Y5P	O4'-C1'-N1-C2
17	AY	29	Y5P	O4'-C1'-N1-C2
17	AV	30	Y5P	O4'-C1'-N1-C2
17	AY	30	Y5P	O4'-C1'-N1-C2
17	AV	31	Y5P	O4'-C1'-N1-C2
17	AY	31	Y5P	O4'-C1'-N1-C2
17	AY	33	Y5P	O4'-C1'-N1-C2
17	AV	37	Y5P	O4'-C1'-N1-C2
17	AY	37	Y5P	O4'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
17	AV	38	Y5P	O4'-C1'-N1-C2
17	AY	38	Y5P	O4'-C1'-N1-C2
17	AV	39	Y5P	O4'-C1'-N1-C2
17	AY	39	Y5P	O4'-C1'-N1-C2
17	AV	40	Y5P	O4'-C1'-N1-C2
17	AY	40	Y5P	O4'-C1'-N1-C2
17	AV	41	Y5P	O4'-C1'-N1-C2
17	AY	41	Y5P	O4'-C1'-N1-C2
17	AY	42	Y5P	O4'-C1'-N1-C2
17	AV	43	Y5P	O4'-C1'-N1-C2
17	AV	44	Y5P	O4'-C1'-N1-C2
17	AY	44	Y5P	O4'-C1'-N1-C2
17	AY	45	Y5P	O4'-C1'-N1-C2
17	AV	49	Y5P	O4'-C1'-N1-C2
17	AV	50	Y5P	O4'-C1'-N1-C2
17	AY	50	Y5P	O4'-C1'-N1-C2
17	AV	51	Y5P	O4'-C1'-N1-C2
17	AY	51	Y5P	O4'-C1'-N1-C2
17	AV	52	Y5P	O4'-C1'-N1-C2
17	AY	52	Y5P	O4'-C1'-N1-C2
17	AY	53	Y5P	O4'-C1'-N1-C2
17	AV	54	Y5P	O4'-C1'-N1-C2
17	AV	57	Y5P	O4'-C1'-N1-C2
17	AV	59	Y5P	O4'-C1'-N1-C2
17	AY	59	Y5P	O4'-C1'-N1-C2
17	AY	62	Y5P	O4'-C1'-N1-C2
17	AV	63	Y5P	O4'-C1'-N1-C2
17	AY	63	Y5P	O4'-C1'-N1-C2
17	AV	64	Y5P	O4'-C1'-N1-C2
17	AV	65	Y5P	O4'-C1'-N1-C2
17	AY	65	Y5P	O4'-C1'-N1-C2
17	AY	67	Y5P	O4'-C1'-N1-C2
17	AV	68	Y5P	O4'-C1'-N1-C2
17	AY	68	Y5P	O4'-C1'-N1-C2
17	AV	69	Y5P	O4'-C1'-N1-C2
17	AY	69	Y5P	O4'-C1'-N1-C2
17	AV	70	Y5P	O4'-C1'-N1-C2
17	AY	70	Y5P	O4'-C1'-N1-C2
17	AV	71	Y5P	O4'-C1'-N1-C2
17	AY	71	Y5P	O4'-C1'-N1-C2
17	AV	72	Y5P	O4'-C1'-N1-C2
17	AY	72	Y5P	O4'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
17	AV	74	Y5P	O4'-C1'-N1-C2
18	AX	15	Y5P	O4'-C1'-N1-C2
18	AX	16	Y5P	O4'-C1'-N1-C2
18	AX	17	Y5P	O4'-C1'-N1-C2
18	AX	19	Y5P	O4'-C1'-N1-C2
18	AX	20	Y5P	O4'-C1'-N1-C2
18	AX	22	Y5P	O4'-C1'-N1-C2
47	BB	8	Y5P	O4'-C1'-N1-C2
47	BB	11	Y5P	O4'-C1'-N1-C2
47	BB	12	Y5P	O4'-C1'-N1-C2
47	BB	13	Y5P	O4'-C1'-N1-C2
47	BB	26	Y5P	O4'-C1'-N1-C2
47	BB	31	Y5P	O4'-C1'-N1-C2
47	BB	33	Y5P	O4'-C1'-N1-C2
47	BB	40	Y5P	O4'-C1'-N1-C2
47	BB	43	Y5P	O4'-C1'-N1-C2
47	BB	44	Y5P	O4'-C1'-N1-C2
47	BB	48	Y5P	O4'-C1'-N1-C2
47	BB	53	Y5P	O4'-C1'-N1-C2
47	BB	60	Y5P	O4'-C1'-N1-C2
47	BB	62	Y5P	O4'-C1'-N1-C2
47	BB	65	Y5P	O4'-C1'-N1-C2
17	AY	73	Y5P	O4'-C1'-N1-C6
47	BB	5	P5P	C3'-C4'-C5'-O5'
47	BB	9	P5P	C3'-C4'-C5'-O5'
47	BB	14	P5P	C3'-C4'-C5'-O5'
47	BB	24	P5P	O4'-C4'-C5'-O5'
47	BB	25	P5P	C3'-C4'-C5'-O5'
47	BB	35	P5P	C3'-C4'-C5'-O5'
17	AV	2	Y5P	O4'-C4'-C5'-O5'
17	AV	6	Y5P	C3'-C4'-C5'-O5'
17	AY	13	Y5P	O4'-C4'-C5'-O5'
17	AV	14	Y5P	O4'-C4'-C5'-O5'
17	AV	14	Y5P	C3'-C4'-C5'-O5'
17	AY	15	Y5P	C3'-C4'-C5'-O5'
17	AY	30	Y5P	C3'-C4'-C5'-O5'
17	AY	37	Y5P	O4'-C4'-C5'-O5'
17	AY	41	Y5P	O4'-C4'-C5'-O5'
17	AY	42	Y5P	O4'-C4'-C5'-O5'
17	AY	42	Y5P	C3'-C4'-C5'-O5'
18	AX	13	Y5P	O4'-C4'-C5'-O5'
18	AX	13	Y5P	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
18	AX	15	Y5P	C3'-C4'-C5'-O5'
47	BB	43	Y5P	O4'-C4'-C5'-O5'
47	BB	43	Y5P	C3'-C4'-C5'-O5'
17	AV	67	Y5P	O4'-C1'-N1-C2
47	BB	34	Y5P	O4'-C1'-N1-C2
17	AV	73	Y5P	O4'-C1'-N1-C6
17	AV	9	Y5P	C2'-C1'-N1-C2
17	AV	58	Y5P	C2'-C1'-N1-C2
47	BB	9	P5P	O4'-C4'-C5'-O5'
47	BB	14	P5P	O4'-C4'-C5'-O5'
17	AV	2	Y5P	C3'-C4'-C5'-O5'
17	AV	7	Y5P	O4'-C4'-C5'-O5'
17	AV	9	Y5P	O4'-C4'-C5'-O5'
17	AV	9	Y5P	C3'-C4'-C5'-O5'
17	AY	9	Y5P	O4'-C4'-C5'-O5'
17	AY	9	Y5P	C3'-C4'-C5'-O5'
17	AY	13	Y5P	C3'-C4'-C5'-O5'
17	AY	37	Y5P	C3'-C4'-C5'-O5'
17	AY	41	Y5P	C3'-C4'-C5'-O5'
17	AY	67	Y5P	O4'-C4'-C5'-O5'
17	AY	67	Y5P	C3'-C4'-C5'-O5'
17	AV	69	Y5P	C3'-C4'-C5'-O5'
17	AV	75	Y5P	C3'-C4'-C5'-O5'
18	AX	23	Y5P	C3'-C4'-C5'-O5'
47	BB	44	Y5P	C3'-C4'-C5'-O5'
47	BB	48	Y5P	C3'-C4'-C5'-O5'
17	AY	58	Y5P	C2'-C1'-N1-C2
18	AX	12	Y5P	O4'-C4'-C5'-O5'
17	AY	58	Y5P	C2'-C1'-N1-C6
18	AX	12	Y5P	C3'-C4'-C5'-O5'
17	AY	34	P5P	C3'-C4'-C5'-O5'
47	BB	15	P5P	C3'-C4'-C5'-O5'
17	AY	21	Y5P	C3'-C4'-C5'-O5'
17	AV	32	Y5P	C3'-C4'-C5'-O5'
17	AV	59	Y5P	C3'-C4'-C5'-O5'
47	BB	12	Y5P	O4'-C4'-C5'-O5'
47	BB	12	Y5P	C3'-C4'-C5'-O5'
17	AV	45	Y5P	O4'-C1'-N1-C2
18	AX	21	Y5P	O4'-C1'-N1-C2
17	AY	73	Y5P	C4'-C5'-O5'-P
17	AY	7	Y5P	O4'-C1'-N1-C2
47	BB	46	P5P	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
17	AY	21	Y5P	O4'-C4'-C5'-O5'
47	BB	34	Y5P	O4'-C4'-C5'-O5'
47	BB	34	Y5P	C3'-C4'-C5'-O5'
17	AV	9	Y5P	O4'-C1'-N1-C6
47	BB	24	P5P	C3'-C4'-C5'-O5'
47	BB	25	P5P	O4'-C4'-C5'-O5'
47	BB	46	P5P	O4'-C4'-C5'-O5'
17	AY	43	Y5P	C3'-C4'-C5'-O5'
17	AV	69	Y5P	O4'-C4'-C5'-O5'
18	AX	15	Y5P	O4'-C4'-C5'-O5'
47	BB	9	P5P	C2'-C1'-N9-C8
17	AY	43	Y5P	O4'-C4'-C5'-O5'
18	AX	16	Y5P	O4'-C4'-C5'-O5'
17	AV	48	Y5P	O4'-C1'-N1-C2
18	AX	16	Y5P	C3'-C4'-C5'-O5'
17	AV	7	Y5P	C3'-C4'-C5'-O5'
17	AV	55	Y5P	O4'-C1'-N1-C2
17	AY	75	Y5P	O4'-C1'-N1-C2
47	BB	9	P5P	C2'-C1'-N9-C4
17	AV	60	Y5P	O4'-C1'-N1-C2
17	AY	58	Y5P	O4'-C1'-N1-C6
17	AY	51	Y5P	C3'-C4'-C5'-O5'
17	AY	61	Y5P	O4'-C4'-C5'-O5'
17	AY	58	Y5P	O4'-C1'-N1-C2
17	AY	52	Y5P	C3'-C4'-C5'-O5'
17	AY	61	Y5P	C3'-C4'-C5'-O5'
17	AY	65	Y5P	O4'-C4'-C5'-O5'
17	AY	56	Y5P	O4'-C1'-N1-C2
18	AX	18	Y5P	O4'-C1'-N1-C2
17	AY	75	Y5P	O4'-C4'-C5'-O5'
18	AX	14	Y5P	O4'-C4'-C5'-O5'
47	BB	5	P5P	C4'-C5'-O5'-P
17	AV	14	Y5P	C2'-C1'-N1-C6
47	BB	46	P5P	C4'-C5'-O5'-P
17	AV	6	Y5P	C4'-C5'-O5'-P
17	AV	49	Y5P	C3'-C4'-C5'-O5'
47	BB	48	Y5P	O4'-C4'-C5'-O5'
17	AV	58	Y5P	O4'-C1'-N1-C6
17	AY	57	Y5P	O4'-C1'-N1-C2
17	AV	75	Y5P	O4'-C1'-N1-C2
17	AY	28	Y5P	C4'-C5'-O5'-P
47	BB	49	P5P	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
17	AV	62	Y5P	C3'-C4'-C5'-O5'
17	AY	60	Y5P	O4'-C1'-N1-C2
47	BB	49	P5P	C3'-C4'-C5'-O5'
17	AY	51	Y5P	O4'-C4'-C5'-O5'
17	AY	55	Y5P	O4'-C1'-N1-C6
18	AX	24	Y5P	O4'-C4'-C5'-O5'
47	BB	7	P5P	C4'-C5'-O5'-P
47	BB	8	Y5P	C4'-C5'-O5'-P
18	AX	17	Y5P	O4'-C4'-C5'-O5'
17	AV	49	Y5P	O4'-C4'-C5'-O5'
17	AV	57	Y5P	C3'-C4'-C5'-O5'
17	AV	14	Y5P	C2'-C1'-N1-C2
17	AY	55	Y5P	C2'-C1'-N1-C6
17	AY	69	Y5P	C2'-C1'-N1-C6
47	BB	23	P5P	C3'-C4'-C5'-O5'
17	AY	30	Y5P	C4'-C5'-O5'-P
47	BB	27	P5P	C2'-C1'-N9-C8
17	AV	58	Y5P	O4'-C1'-N1-C2
17	AY	60	Y5P	C2'-C1'-N1-C2
17	AV	37	Y5P	O4'-C4'-C5'-O5'
17	AY	65	Y5P	C3'-C4'-C5'-O5'
17	AY	23	Y5P	C4'-C5'-O5'-P
17	AY	37	Y5P	C2'-C1'-N1-C6
17	AY	59	Y5P	O4'-C4'-C5'-O5'

There are no ring outliers.

140 monomers are involved in 187 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	AX	12	Y5P	1	0
17	AV	12	Y5P	1	0
17	AV	67	Y5P	4	0
47	BB	37	P5P	2	0
17	AV	52	Y5P	2	0
17	AY	37	Y5P	3	0
17	AY	29	Y5P	2	0
17	AV	13	Y5P	1	0
17	AY	30	Y5P	2	0
17	AV	66	Y5P	3	0
18	AX	17	Y5P	1	0
17	AV	49	Y5P	1	0
17	AV	24	Y5P	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	AY	33	Y5P	2	0
47	BB	9	P5P	2	0
18	AX	22	Y5P	1	0
17	AV	29	Y5P	4	0
47	BB	11	Y5P	1	0
17	AV	65	Y5P	1	0
17	AY	51	Y5P	1	0
17	AV	33	Y5P	1	0
17	AV	68	Y5P	1	0
17	AV	2	Y5P	2	0
17	AY	44	Y5P	1	0
18	AX	16	Y5P	1	0
17	AV	31	Y5P	2	0
47	BB	29	P5P	3	0
17	AV	21	Y5P	1	0
17	AY	2	Y5P	1	0
17	AY	66	Y5P	1	0
17	AY	27	Y5P	1	0
17	AV	44	Y5P	4	0
47	BB	63	Y5P	1	0
47	BB	36	P5P	1	0
17	AV	5	Y5P	1	0
17	AV	4	Y5P	1	0
17	AY	6	Y5P	3	0
17	AV	54	Y5P	6	0
17	AY	32	Y5P	4	0
17	AY	15	Y5P	1	0
17	AY	61	Y5P	1	0
47	BB	43	Y5P	2	0
17	AY	62	Y5P	2	0
47	BB	25	P5P	3	0
17	AV	27	Y5P	4	0
17	AY	43	Y5P	2	0
47	BB	34	Y5P	1	0
17	AV	9	Y5P	2	0
47	BB	32	P5P	1	0
17	AY	52	Y5P	1	0
17	AV	10	Y5P	4	0
17	AV	25	Y5P	3	0
17	AV	30	Y5P	3	0
17	AY	39	Y5P	2	0
17	AY	53	Y5P	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	AY	4	Y5P	1	0
17	AY	12	Y5P	1	0
17	AY	70	Y5P	2	0
17	AV	53	Y5P	2	0
17	AY	14	Y5P	6	0
17	AY	28	Y5P	2	0
17	AV	26	Y5P	2	0
17	AY	63	Y5P	1	0
47	BB	39	P5P	2	0
47	BB	30	P5P	3	0
17	AV	35	P5P	1	0
47	BB	61	Y5P	2	0
17	AY	45	Y5P	1	0
17	AV	14	Y5P	1	0
17	AY	50	Y5P	1	0
17	AY	74	Y5P	2	0
17	AY	38	Y5P	3	0
18	AX	20	Y5P	1	0
17	AY	9	Y5P	6	0
47	BB	45	P5P	1	0
17	AV	38	Y5P	4	0
17	AY	22	Y5P	6	0
47	BB	33	Y5P	2	0
17	AV	50	Y5P	1	0
18	AX	21	Y5P	3	0
47	BB	31	Y5P	1	0
17	AV	43	Y5P	6	0
47	BB	38	P5P	2	0
17	AV	51	Y5P	2	0
17	AV	36	P5P	2	0
47	BB	46	P5P	1	0
17	AY	11	Y5P	2	0
17	AY	71	Y5P	2	0
47	BB	62	Y5P	3	0
47	BB	44	Y5P	3	0
17	AV	11	Y5P	2	0
17	AV	48	Y5P	2	0
17	AY	7	Y5P	2	0
17	AY	55	Y5P	14	0
47	BB	12	Y5P	1	0
17	AV	71	Y5P	1	0
17	AY	34	P5P	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	AY	36	P5P	2	0
17	AV	8	Y5P	1	0
17	AY	25	Y5P	6	0
17	AY	8	Y5P	5	0
17	AV	55	Y5P	7	0
17	AY	67	Y5P	3	0
17	AY	3	Y5P	3	0
17	AV	59	Y5P	2	0
17	AV	58	Y5P	4	0
17	AY	31	Y5P	3	0
47	BB	48	Y5P	1	0
47	BB	24	P5P	4	0
47	BB	13	Y5P	2	0
17	AV	63	Y5P	4	0
17	AV	62	Y5P	2	0
17	AV	41	Y5P	1	0
47	BB	26	Y5P	2	0
17	AY	24	Y5P	3	0
17	AV	37	Y5P	5	0
17	AY	68	Y5P	4	0
17	AY	56	Y5P	1	0
47	BB	47	P5P	1	0
17	AV	60	Y5P	2	0
17	AY	23	Y5P	1	0
18	AX	18	Y5P	2	0
17	AY	58	Y5P	11	0
17	AY	69	Y5P	2	0
17	AY	57	Y5P	3	0
17	AV	34	P5P	1	0
17	AV	57	Y5P	5	0
47	BB	65	Y5P	2	0
47	BB	28	P5P	3	0
17	AY	26	Y5P	3	0
47	BB	23	P5P	1	0
17	AY	42	Y5P	1	0
17	AV	3	Y5P	1	0
17	AV	64	Y5P	3	0
17	AY	54	Y5P	6	0
17	AV	32	Y5P	1	0
17	AV	42	Y5P	3	0
17	AV	70	Y5P	1	0
17	AV	28	Y5P	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
47	BB	66	P5P	2	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 358 ligands modelled in this entry, 357 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
91	GDP	Ag	500	-	29,30,30	1.35	2 (6%)	45,47,47	1.88	6 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
91	GDP	Ag	500	-	-	7/16/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
91	Ag	500	GDP	PA-O3A	3.73	1.63	1.59
91	Ag	500	GDP	C5-C4	3.65	1.48	1.38

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
91	Ag	500	GDP	C5-C4-N3	-6.42	118.18	128.39
91	Ag	500	GDP	C2-N3-C4	5.36	121.53	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
91	Ag	500	GDP	N9-C4-N3	4.71	135.38	125.95
91	Ag	500	GDP	C6-C5-N7	3.26	136.23	130.29
91	Ag	500	GDP	C4-C5-N7	-2.65	106.47	110.67
91	Ag	500	GDP	C3'-C2'-C1'	2.14	105.51	101.46

There are no chirality outliers.

All (7) torsion outliers are listed below:

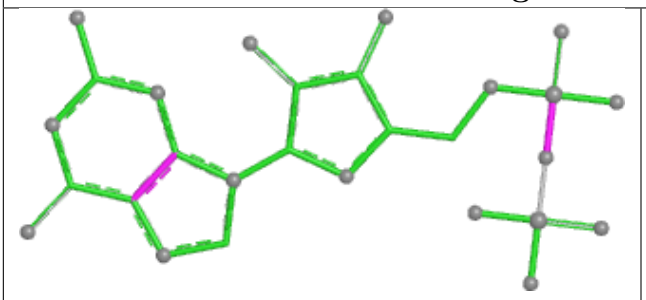
Mol	Chain	Res	Type	Atoms
91	Ag	500	GDP	C5'-O5'-PA-O3A
91	Ag	500	GDP	C5'-O5'-PA-O1A
91	Ag	500	GDP	C5'-O5'-PA-O2A
91	Ag	500	GDP	O4'-C4'-C5'-O5'
91	Ag	500	GDP	C3'-C4'-C5'-O5'
91	Ag	500	GDP	PB-O3A-PA-O2A
91	Ag	500	GDP	PB-O3A-PA-O1A

There are no ring outliers.

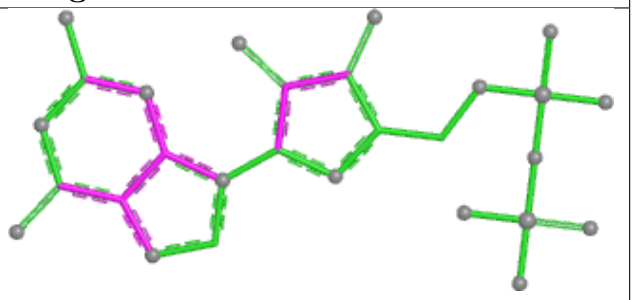
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

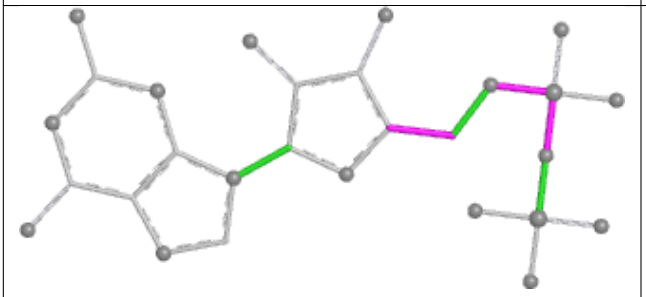
Ligand GDP Ag 500



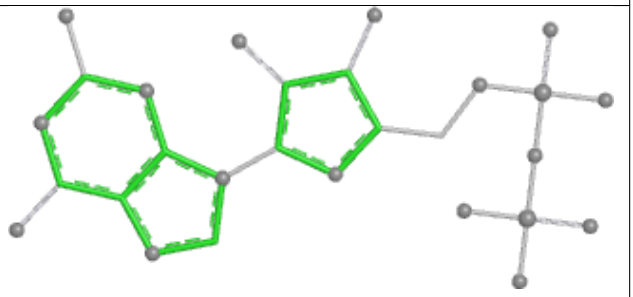
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
32	Ao	26
88	Bz	4
23	Ae	4
17	AY	3
47	BB	2
17	AV	2
7	AI	1
4	AE	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Bz	36:UNK	C	99:UNK	N	56.86
1	Bz	425:UNK	C	601:UNK	N	55.59
1	Ae	262:UNK	C	263:UNK	N	42.03
1	Ae	309:UNK	C	354:UNK	N	28.87

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Bz	106:UNK	C	300:UNK	N	28.46
1	AI	177:ASN	C	195:PRO	N	26.78
1	Ao	143:GLU	C	153:UNK	N	24.92
1	Bz	315:UNK	C	399:UNK	N	22.81
1	Ao	405:UNK	C	410:UNK	N	21.39
1	BB	53:Y5P	O3'	58:P5P	P	17.94
1	Ao	368:UNK	C	371:UNK	N	16.08
1	AE	106:SER	C	122:ARG	N	16.04
1	AV	15:Y5P	O3'	21:Y5P	P	14.94
1	AY	15:Y5P	O3'	21:Y5P	P	14.74
1	Ao	292:UNK	C	295:UNK	N	14.07
1	Ao	250:UNK	C	260:UNK	N	13.92
1	Ao	181:UNK	C	185:UNK	N	13.52
1	Ao	349:UNK	C	355:UNK	N	13.13
1	Ae	292:UNK	C	293:UNK	N	12.58
1	Ao	607:UNK	C	651:UNK	N	12.48
1	Ao	585:UNK	C	593:UNK	N	12.31
1	Ao	310:UNK	C	315:UNK	N	11.71
1	Ao	215:UNK	C	220:UNK	N	11.36
1	Ao	330:UNK	C	335:UNK	N	11.30
1	Ao	560:UNK	C	575:UNK	N	11.29
1	Ao	447:UNK	C	456:UNK	N	11.26
1	AY	45:Y5P	O3'	48:Y5P	P	10.79
1	Ao	198:UNK	C	200:UNK	N	10.76
1	Ao	661:UNK	C	666:UNK	N	10.72
1	BB	15:P5P	O3'	23:P5P	P	9.76
1	Ao	275:UNK	C	277:UNK	N	9.70
1	Ae	211:UNK	C	212:UNK	N	9.63
1	Ao	490:UNK	C	492:UNK	N	9.62
1	AV	45:Y5P	O3'	48:Y5P	P	9.50
1	Ao	525:UNK	C	531:UNK	N	9.11
1	Ao	470:UNK	C	475:UNK	N	8.37
1	Ao	235:UNK	C	237:UNK	N	7.59
1	Ao	385:UNK	C	390:UNK	N	7.45
1	Ao	165:UNK	C	167:UNK	N	6.98
1	Ao	507:UNK	C	510:UNK	N	6.97
1	Ao	430:UNK	C	433:UNK	N	6.37
1	Ao	542:UNK	C	546:UNK	N	5.15
1	AY	7:Y5P	O3'	8:Y5P	P	3.72

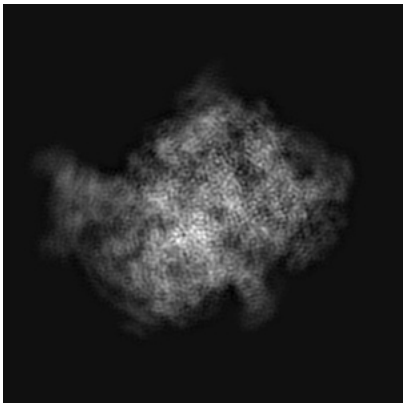
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-2914. These allow visual inspection of the internal detail of the map and identification of artifacts.

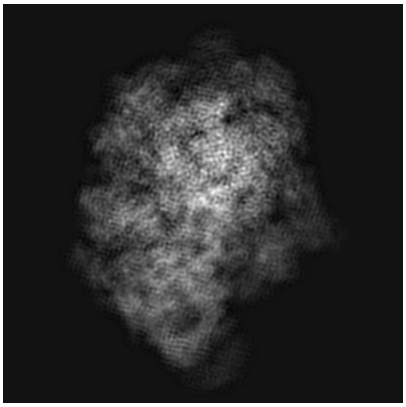
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

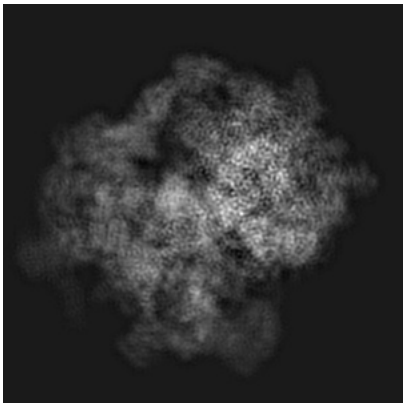
6.1.1 Primary map



X



Y

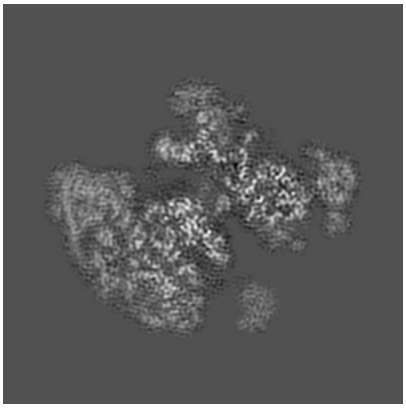


Z

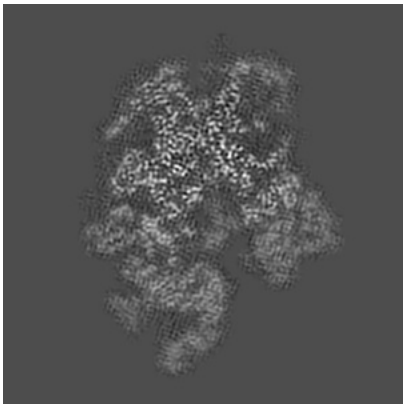
The images above show the map projected in three orthogonal directions.

6.2 Central slices

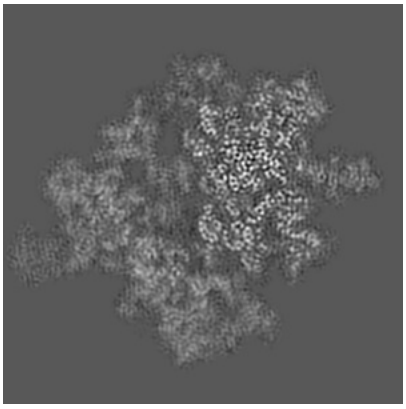
6.2.1 Primary map



X Index: 128



Y Index: 128

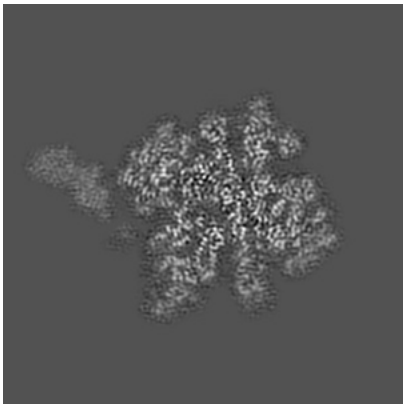


Z Index: 128

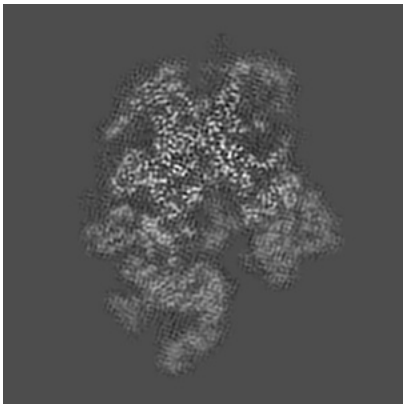
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

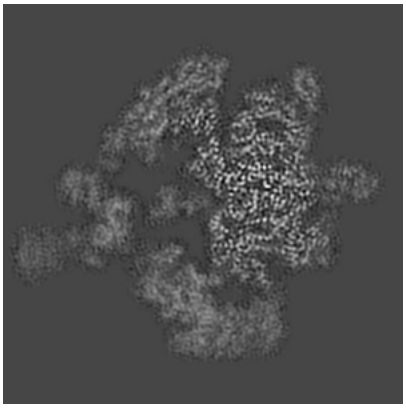
6.3.1 Primary map



X Index: 159



Y Index: 128

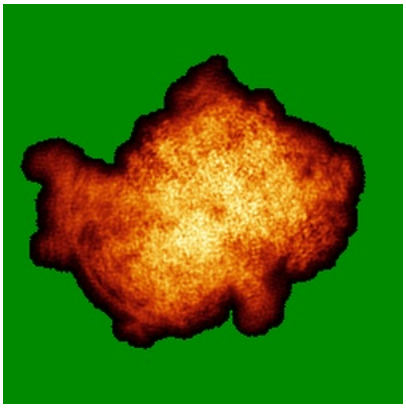


Z Index: 138

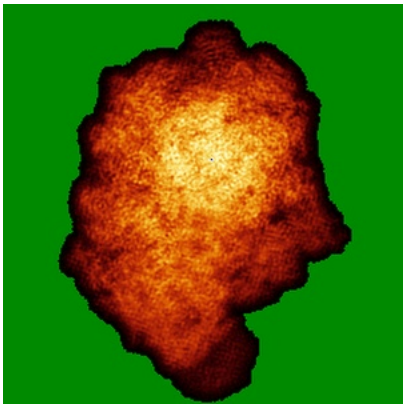
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

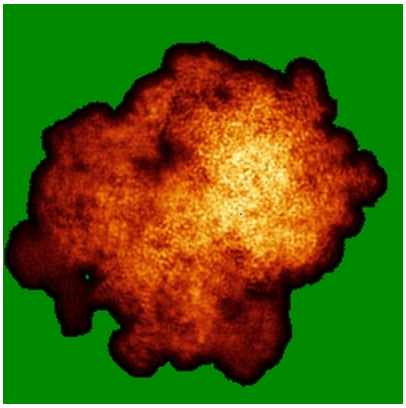
6.4.1 Primary map



X



Y

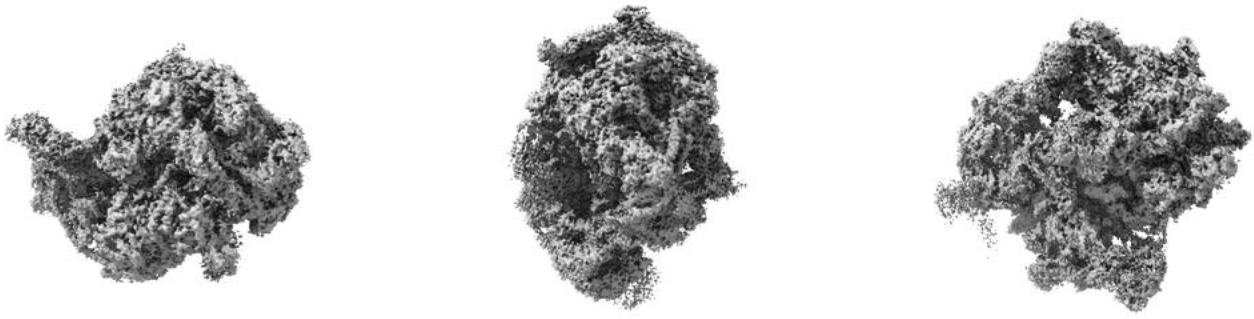


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

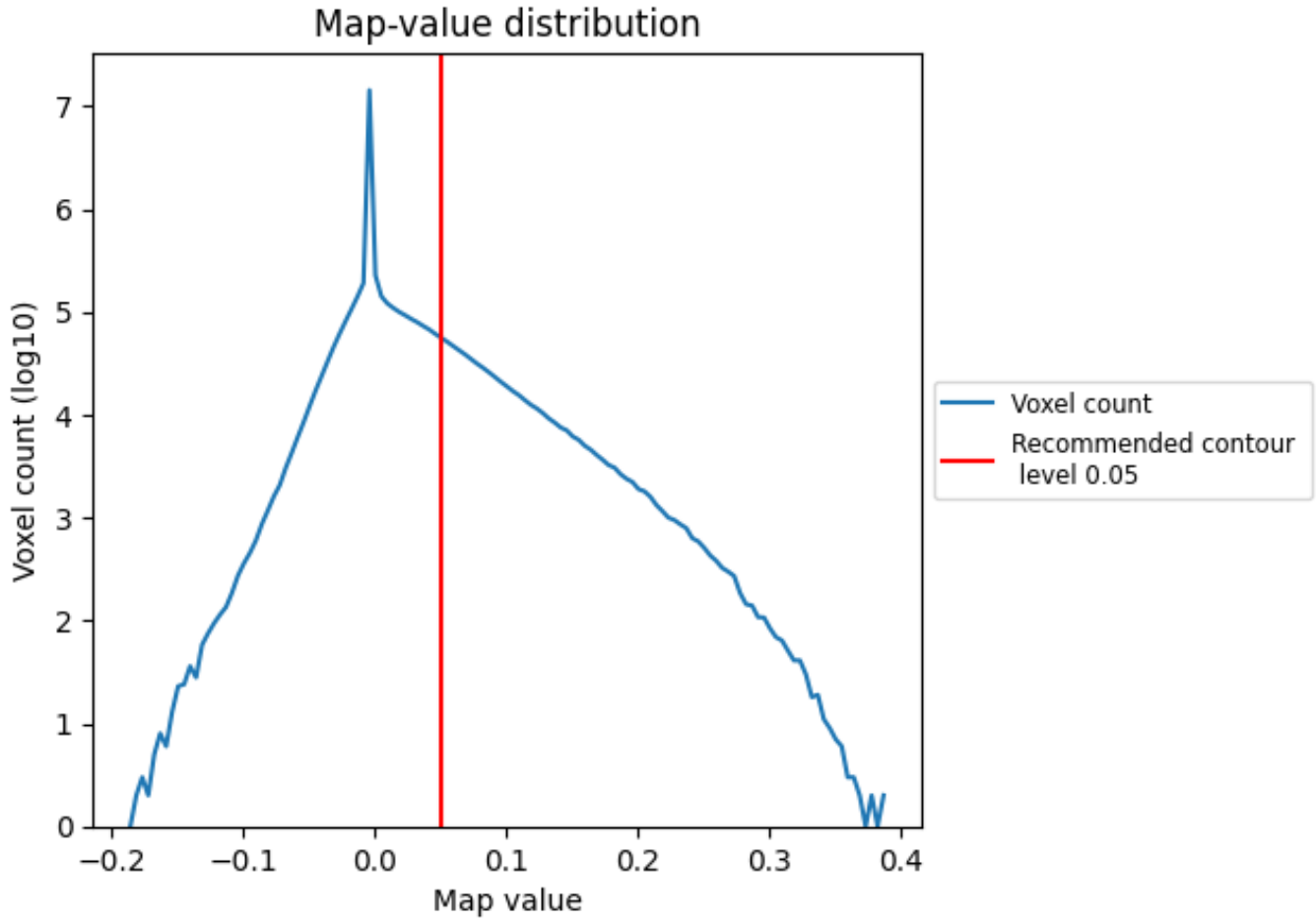
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

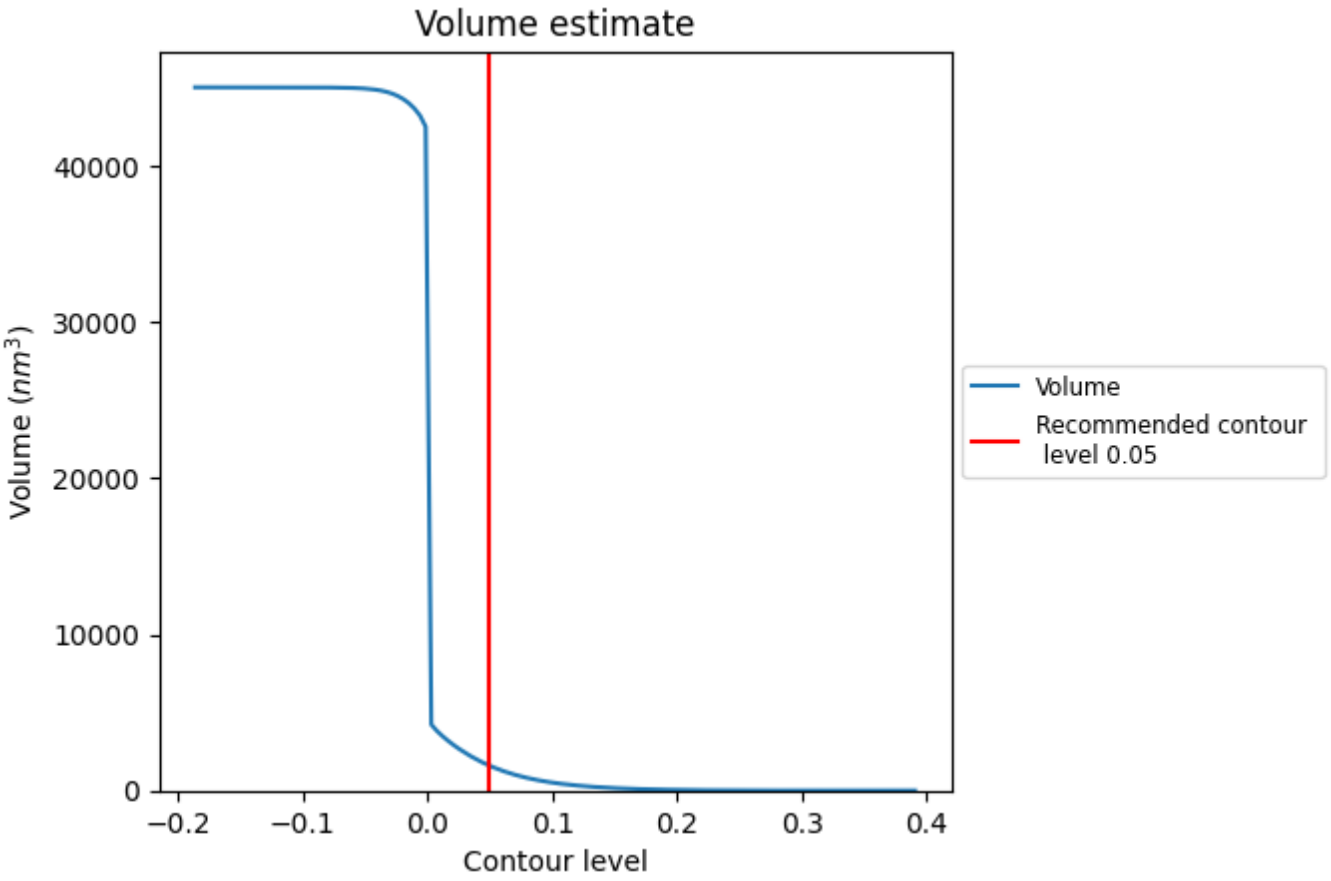
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

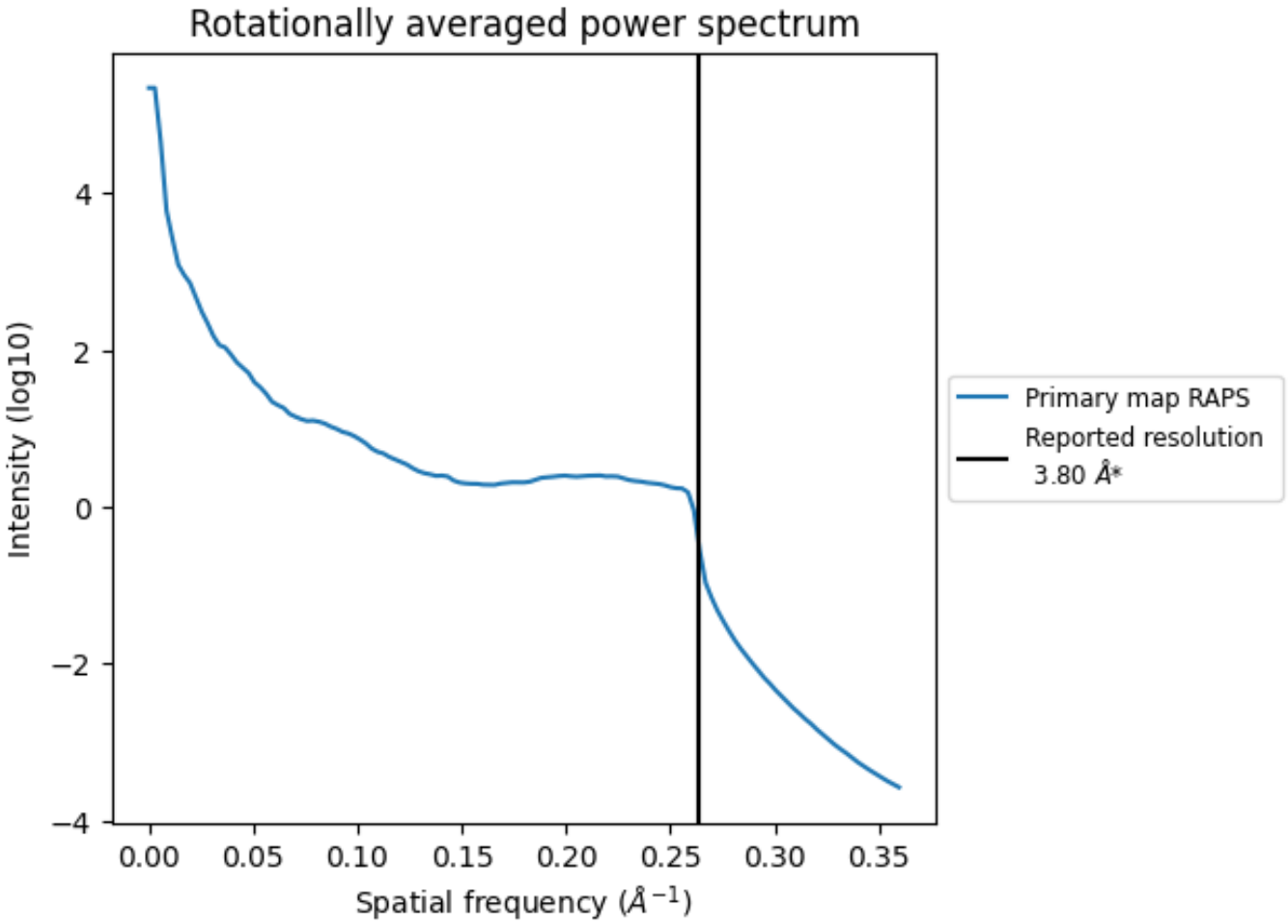
7.2 Volume estimate



The volume at the recommended contour level is 1591 nm^3; this corresponds to an approximate mass of 1437 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

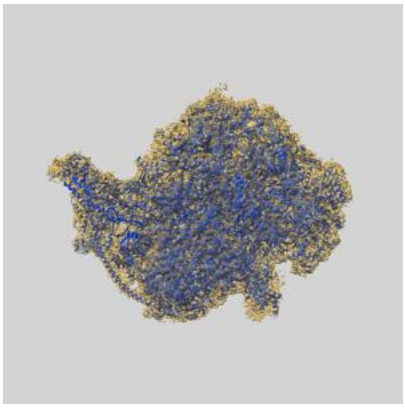
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

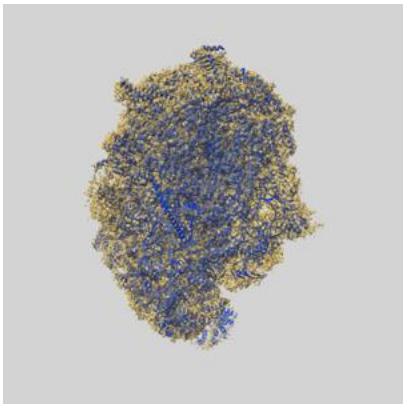
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-2914 and PDB model 5AJ4. Per-residue inclusion information can be found in section 3 on page 23.

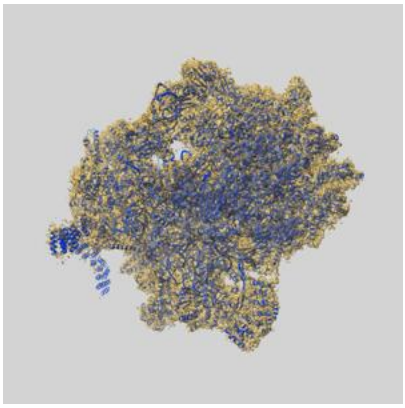
9.1 Map-model overlay



X



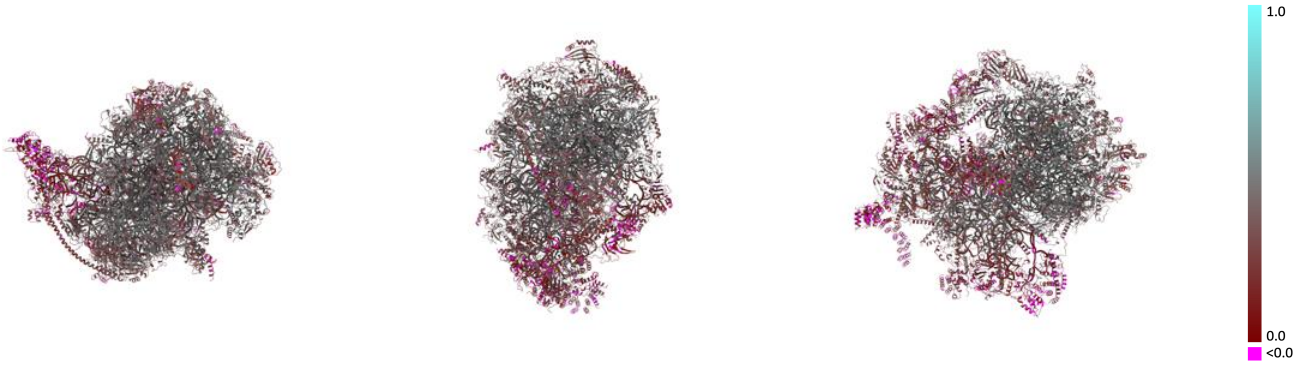
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

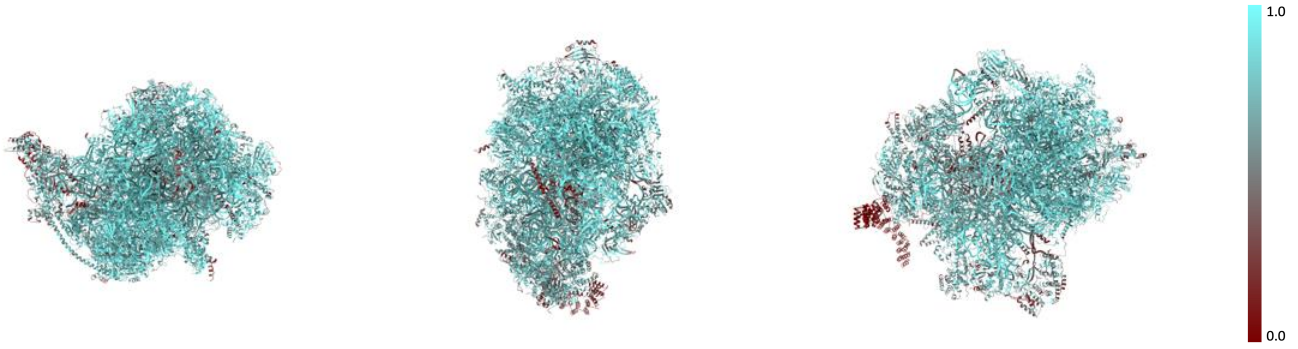
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

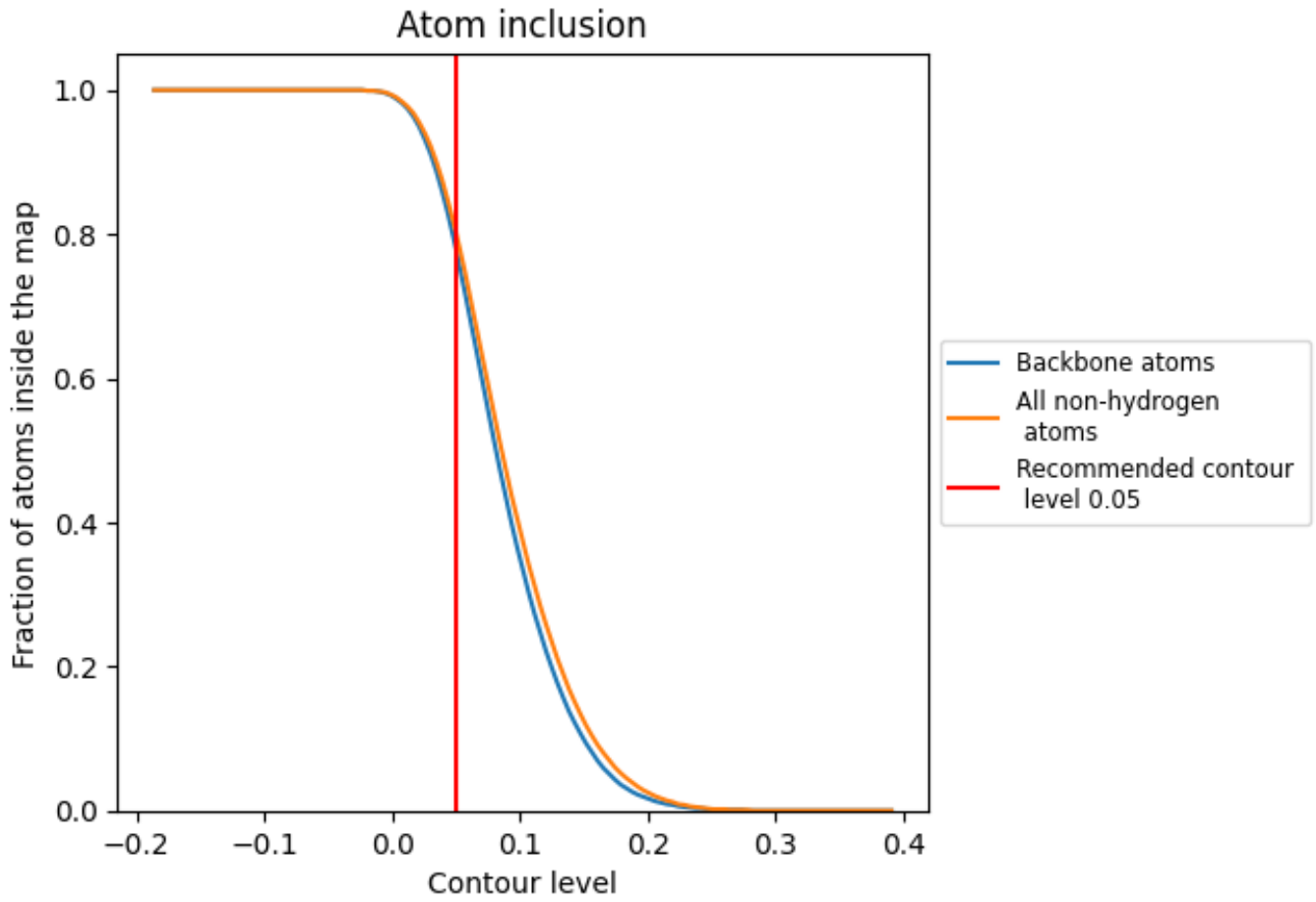
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8030	0.3580
AA	0.9200	0.3580
AB	0.7920	0.3500
AC	0.7490	0.3540
AE	0.7070	0.3400
AF	0.7510	0.3610
AG	0.6430	0.2620
AI	0.7100	0.2850
AJ	0.7180	0.2990
AK	0.8160	0.3670
AL	0.7460	0.3790
AN	0.7890	0.3120
AO	0.7150	0.3430
AP	0.7240	0.2080
AQ	0.7940	0.3420
AR	0.7900	0.3810
AU	0.7950	0.3760
AV	0.6410	0.2940
AX	0.7490	0.4000
AY	0.4840	0.2070
Aa	0.6410	0.1880
Ab	0.6870	0.2790
Ac	0.7380	0.3080
Ad	0.7310	0.2440
Ae	0.5250	0.1220
Af	0.7290	0.3360
Ag	0.6800	0.1920
Ah	0.6970	0.2250
Ai	0.7280	0.2650
Aj	0.5360	0.1580
Ak	0.6560	0.2400
Am	0.6970	0.3340
An	0.7910	0.4160
Ao	0.2110	0.1440
Ap	0.7260	0.2400

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Chain	Atom inclusion	Q-score
As	0.0730	-0.0030
Az	0.7550	0.2900
B0	0.9010	0.4720
B1	0.8310	0.4060
B2	0.8590	0.4290
B3	0.8860	0.4520
B4	0.8340	0.2750
B5	0.8490	0.4260
B6	0.1900	0.1820
B7	0.9080	0.4800
B8	0.8970	0.4840
B9	0.9250	0.4600
BA	0.9540	0.4350
BB	0.8950	0.2640
BD	0.8810	0.4570
BE	0.8710	0.4320
BF	0.8920	0.4530
BI	0.7290	0.3510
BJ	0.6380	0.2690
BK	0.4930	0.1750
BN	0.8910	0.4580
BO	0.8690	0.4550
BP	0.8990	0.4400
BQ	0.8740	0.4420
BR	0.8780	0.4480
BS	0.8560	0.3790
BT	0.8230	0.4230
BU	0.8710	0.4490
BV	0.8490	0.4390
BW	0.8590	0.4720
BX	0.8510	0.4360
BY	0.6230	0.3490
Ba	0.8690	0.4050
Bb	0.8340	0.3330
Bc	0.8180	0.3520
Bd	0.7260	0.2320
Be	0.8260	0.3880
Bf	0.7790	0.4070
Bg	0.8900	0.4590
Bh	0.8320	0.3890
Bi	0.5600	0.2960
Bj	0.7040	0.1810

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Chain	Atom inclusion	Q-score
Bk	0.7420	0.3210
Bl	0.8990	0.4350
Bm	0.7690	0.3240
Bn	0.8900	0.4730
Bo	0.8610	0.4180
Bp	0.5970	0.2170
Bq	0.6390	0.2510
Bt	0.8870	0.4650
Bu	0.5420	0.2520
Bv	0.5470	0.2740
Bw	0.8630	0.4070
Bx	0.8200	0.3960
Bz	0.3940	0.2010